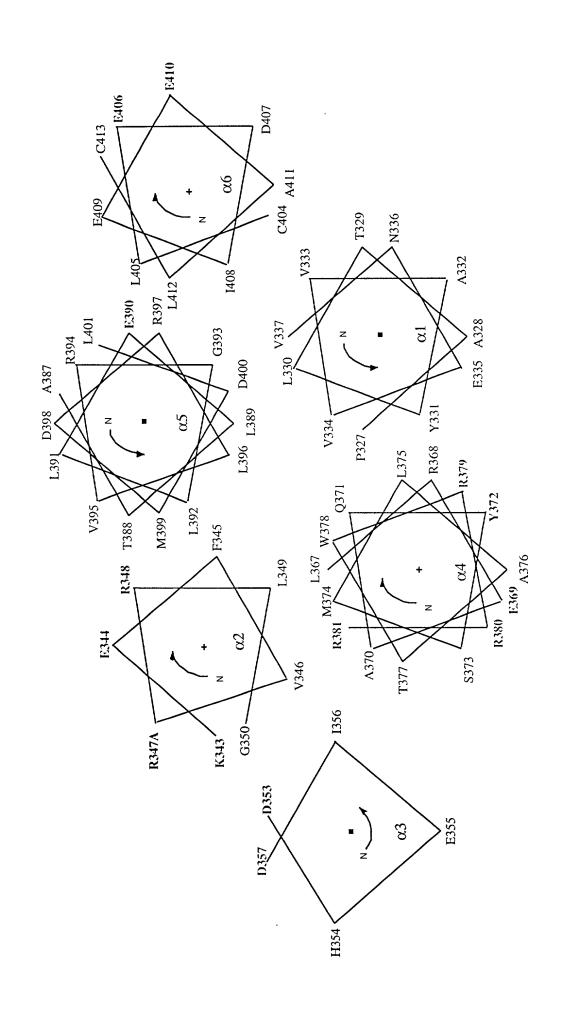
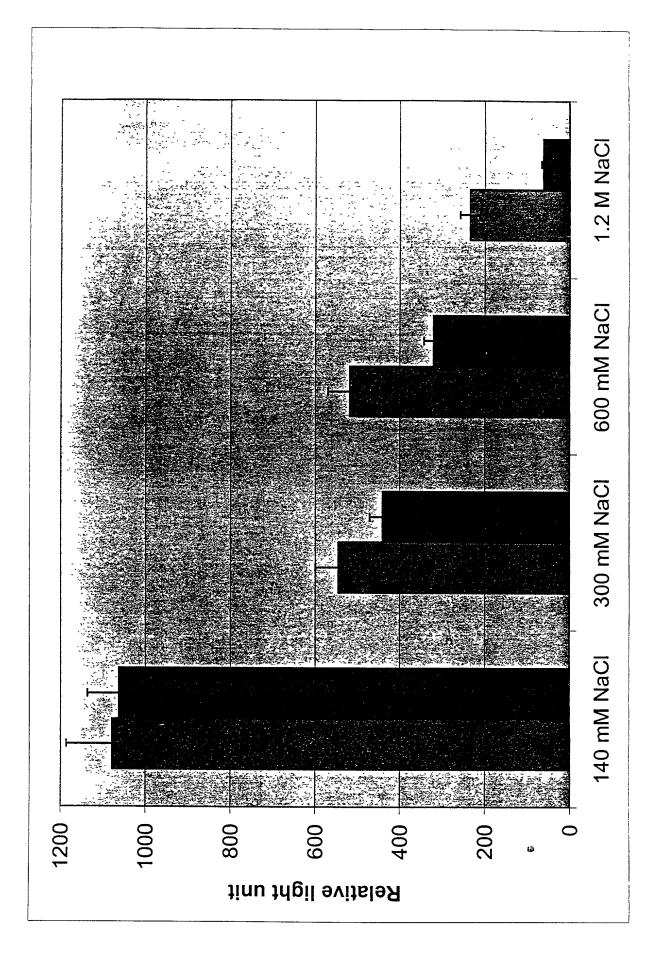
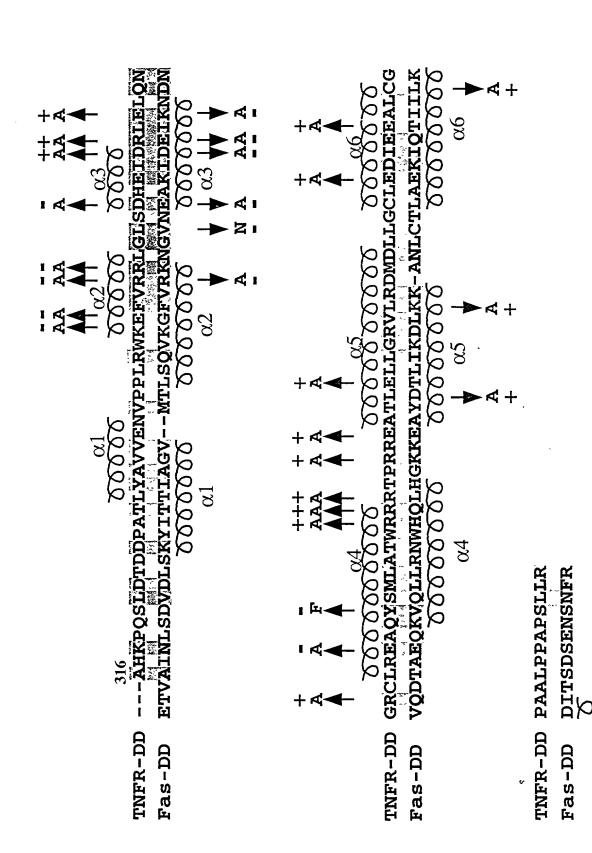
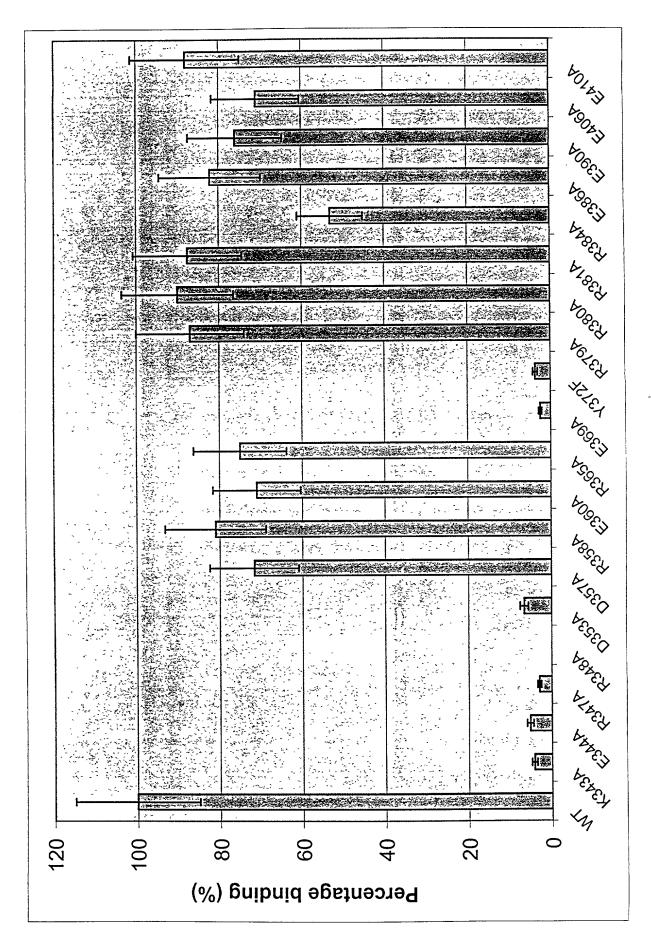
320 330 340 350 360 380 380 380 370 380 MAHKPQSLDTDDPATLYAVVENVPPLRWKEFVARLGLSDHEIDRLELQNGRCLREAQYSMLATWRRR rereservers α4 TPRREATLELLGRVLRDMDLLGCLEDIEEALCGPAALFPAPSLLR arres  $\alpha_3$ Full II will make 1 222222 reserves 000000 α 100 400  $\Delta^{13}C\alpha \text{ (ppm)} \stackrel{+4}{\overset{-4}{0}}$   $\Delta^{13}C\beta \text{ (ppm)} \stackrel{0}{\overset{+4}{0}}$  $\Delta^{13}C\beta$  (ppin) 0.4 $\Lambda^{13}C\alpha \text{ (ppm)} \stackrel{+4}{0}$  $^{3}$ HIN $\alpha(<5$ Hz)  $^{3J}$ HN $\alpha$ (<5Hz) dαN(i,i+3) dαN(i,i+4)  $^{\mathrm{d}}\alpha\mathrm{N}(\mathrm{i},\mathrm{i+1})$ dNN(i,i+1) dβN(i,i+1) dαN(i,i+2) dNN(i,i+2) dαβ(i,i+3) dNN(i,i+2)  $d_{\alpha N(i,i+3)}$  $d_{\alpha N(i,i+4)}$  $d_{\alpha N(i,i+1)}$ dNN(i,i+1) dβN(i,i+1)  $^{\mathrm{d}_{\alpha\beta(i,i+3)}}$ <sup>d</sup>αN(i,i+2)

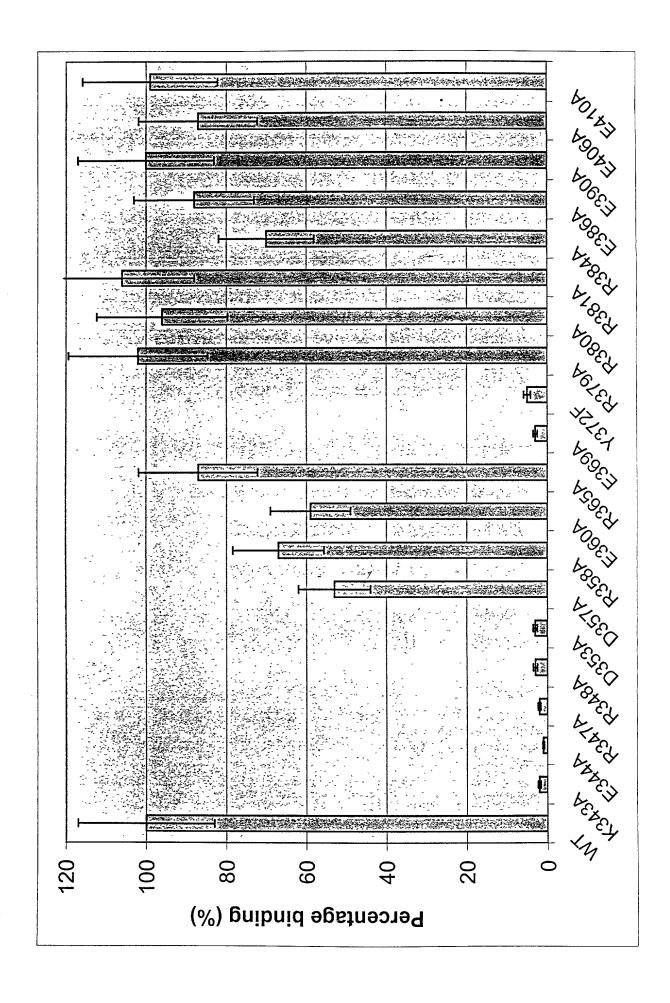
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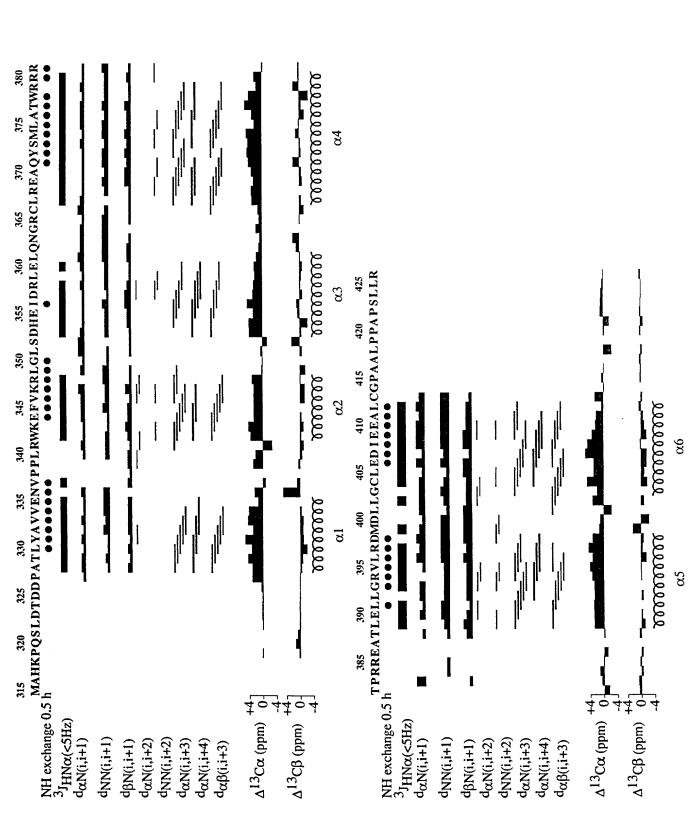




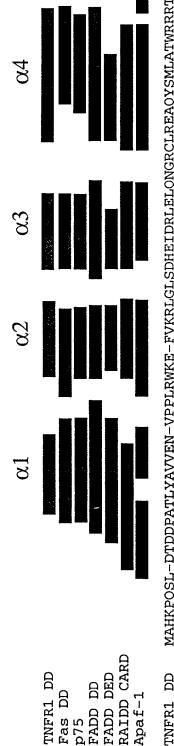


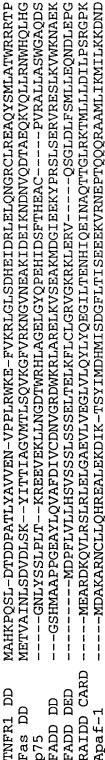






Secondary Structure Indicators of TNFR-DD R347K Summary of



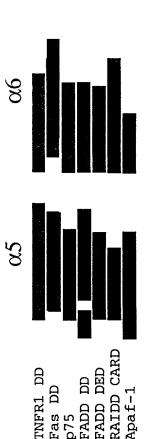


FADD DED

Apaf-1

FADD DD

Fas DD





--AFDTFLDS--LQEF-PWVREKLKKAREEAMTDLPAG SYVSFYNALLHEGY----KDLAALLHDGIPVVSSS HTELLRELLASL----RRHDLLRRVDDFELE RAIDD CARD FADD DED Apaf-1

	Atom Type Residue	Res. No.	Х	Υ	Z		
MOTA	1 N PRO	327	2.816	0.502	11.316	1.00	0.61
MOTA	2 CA PRO	327	2.189	1.819	11.030	1.00	0.60
MOTA MOTA	3 HA PRO 4 CB PRO	327 327	1.287 1.855	1.695 2.377	10.452 12.410	1.00	0.62
ATOM	5 HB1 PRO	327	0.841	2.129	12.681	1.00	0.75
ATOM	6 HB2 PRO	327	2.000	3.449	12.426	1.00	0.68
MOTA	7 CG PRO	327	2.811	1.705	13.337	1.00	0.71
MOTA	8 HG1 PRO 9 HG2 PRO	327 327	2.360 3.718	1.585 2.289	14.310 13.417	1.00 1.00	0.79 0.69
MOTA MOTA	9 HG2 PRO 10 CD PRO	327	3.718	0.354	12.749	1.00	0.68
ATOM	11 HD2 PRO	327	4.156	0.104	12.897	1.00	0.67
MOTA	12 HD1 PRO	327	2.477	-0.400	13.184	1.00	0.74
MOTA MOTA	13 C PRO 14 O PRO	327 327	3.178 2.851	2.733 3.350	10.300 9.306	1.00 1.00	0.51 0.47
MOTA	14 O PRO 15 N ALA	328	4.385	2.823	10.787	1.00	0.51
ATOM	16 HN ALA	328	4.629	2.318	11.591	1.00	0.55
MOTA MOTA	17 CA ALA 18 HA ALA	328 328	5.393 5.006	3.697 4.703	10.123 10.052	1.00	0.46
MOTA	18 HA ALA 19 CB ALA	328	6.684	3.703	10.032	1.00	0.47
ATOM	20 HB1 ALA	328	6.619	4.461	11.711	1.00	1.19
MOTA	21 HB2 ALA	328	7.521	3.917	10.297	1.00	1.04
ATOM ATOM	22 HB3 ALA 23 C ALA	328 328	6.823 5.685	2.736 3.165	11.404 8.720	1.00 1.00	1.17 0.39
ATOM	24 O ALA	328	5.930	3.920	7.799	1.00	0.36
ATOM	25 N THR	329	5.660	1.872	8.545	1.00	0.37
MOTA MOTA	26 HN THR 27 CA THR	329 329	5.459 5.935	1.278 1.303	9.298 7.196	1.00	0.40
ATOM	28 HA THR	329	6.871	1.692	6.823	1.00	0.34
MOTA	29 CB THR	329	6.012	-0.222	7.279	1.00	0.37
MOTA	30 HB THR	329	5.045	-0.618	7.549	1.00	0.40
M <u>Ö</u> TA M <del>Q</del> TA	31 OG1 THR 32 HG1 THR	329 329	6.971 6.878	-0.601 -0.012	8.256 9.009	1.00	0.39
MOTA	33 CG2 THR	329	6.419	-0.779	5.915	1.00	0.38
MOTA	34 HG21 THR	329	6.796	0.023	5.297	1.00	1.08
ATOM ATOM	35 HG22 THR 36 HG23 THR	329 329	5.559 7.188	-1.226 -1.525	5.438 6.044	1.00 1.00	1.05 1.09
MOTA	37 C THR	329	4.804	1.694	6.247	1.00	0.32
MOTA	38 O THR	329	4.984	1.773	5.048	1.00	0.30
MOTA MOTA	39 N LEU 40 HN LEU	330 330	3.638 3.515	1.938 1.868	6.776 7.745	1.00 1.00	0.35
ATOM	40 AN LEU	330	2.495	2.322	5.905	1.00	0.39
MOTA	42 HA LEU	330	2.474	1.678	5.038	1.00	0.36
MÖTA M <del>O</del> TA	43 CB LEU	330	1.175	2.181	6.678	1.00	0.43
ATOM	44 HB1 LEU 45 HB2 LEU	330 330	0.356 1.038	2.118 3.047	5.977 7.309	1.00	0.48
MOTA	46 CG LEU	330	1.193	0.915	7.550	1.00	0.70
ATOM	47 HG LEU	330	1.892	1.049	8.362	1.00	1.17
MOTA MOTA	48 CD1 LEU 49 HD11 LEU	330 330	-0.204 -0.847	0.675 1.504	8.123 7.863	1.00	1.17 1.71
ATOM	50 HD12 LEU	330	-0.142	0.591	9.198	1.00	1.79
MOTA	51 HD13 LEU	330	-0.610	-0.238	7.713	1.00	1.63
MOTA MOTA	52 CD2 LEU 53 HD21 LEU	330 330	1.609 1.114	-0.300 -0.263	6.710 5.752	1.00	1.69 2.25
MOTA	54 HD22 LEU	330	1.327	-1.206	7.226	1.00	2.18
MOTA	55 HD23 LEU	330	2.679	-0.287	6.563	1.00	2.16
MOTA MOTA	56 C LEU 57 O LEU	330 330	2.677 2.472	3.771 4.104	5.454 4.305	1.00	0.33
ATOM	58 N TYR	331	3.074	4.636	6.348	1.00	0.35
MOTA	59 HN TYR	331	3.244	4.347	7.270	1.00	0.38
MOTA MOTA	60 CA TYR 61 HA TYR	331 331	3.281 2.368	6.059 6.457	5.962 5.544	1.00	0.36
MOTA	62 CB TYR	331	3.681	6.872	7.195	1.00	0.37
MOTA	63 HB1 TYR	331	3.987	7.861	6.889	1.00	0.43
MOTA MOTA	64 HB2 TYR 65 CG TYR	331	4.500	6.381	7.699	1.00	0.42
MOTA	65 CG TYR 66 CD1 TYR	331 331	2.504 1.305	6.979 7.551	8.134 7.692	1.00 1.00	0.48 1.26
MOTA	67 HD1 TYR	331	1.221	7.915	6.679	1.00	2.13
MOTA	68 CD2 TYR	331	2.612	6.507	9.448	1.00	1.36
MOTA MOTA	69 HD2 TYR 70 CE1 TYR	331 331	3.538 0.214	6.066 7.650	9.789 8.564	1.00	2.24
MOTA	70 CEI TIR 71 HE1 TYR	331	-0.711	8.091	8.223	1.00	2.18
MOTA	72 CE2 TYR	331	1.521	6.607	10.320	1.00	1.38
MOTA MOTA	73 HE2 TYR 74 CZ TYR	331 331	1.605 0.322	6.243 7.178	11.333 9.878	1.00	2.26
MOTA	75 OH TYR	331	-0.753	7.178	10.737	1.00	0.63 0.71
MOTA	76 HH TYR	331	-0.454	7.713	11.538	1.00	1.10
MOTA	77 C TYR	331	4.396	6.132	4.920	1.00	0.32

ATOM	78 O T	YR 331	4.401	6.986	4.055	1.00	0.33
MOTA	79 N AI	LA 332	5.340	5.235	4.995	1.00	0.31
MOTA		LA 332	5.312	4.555	5.700	1.00	0.33
MOTA	-	LA 332	6.456	5.241	4.011	1.00	0.31
MOTA		LA 332	6.880	6.232	3.950	1.00	0.35
MOTA		LA 332	7.532	4.247 3.281	4.454 4.628	1.00 1.00	0.35 1.08
MOTA	84 HB1 AI		7.081 7.996	4.597	5.363	1.00	0.98
MOTA	85 HB2 A1 86 HB3 A1		8.279	4.160	3.680	1.00	1.12
ATOM ATOM		LA 332	5.922	4.826	2.642	1.00	0.28
MOTA		LA 332	6.274	5.395	1.629	1.00	0.31
ATOM		AL 333	5.077	3.832	2.604	1.00	0.26
MOTA		AL 333	4.809	3.385	3.434	1.00	0.27
MOTA		AL 333	4.525	3.374	1.300	1.00	0.26
MOTA	92 HA V	AL 333	5.335	3.242	0.597	1.00	0.29
MOTA	93 CB V	AL 333	3.803	2.040	1.496	1.00	0.28
ATOM		AL 333	3.015	2.161	2.225	1.00	0.27
ATOM	95 CG1 V		3.202	1.576	0.167	1.00	0.30
ATOM	96 HG11 V		2.209	1.186 0.802	0.338 -0.258	$1.00 \\ 1.00$	1.07 1.01
ATOM	97 HG12 VX 98 HG13 VX		3.823 3.148	2.409	-0.517	1.00	1.09
ATOM ATOM	98 HG13 V 99 CG2 V		4.803	0.993	1.992	1.00	0.33
MOTA	100 HG21 V		5.237	0.480	1.146	1.00	1.10
MOTA	101 HG22 V		4.295	0.279	2.623	1.00	1.02
ATOM	102 HG23 V		5.584	1.481	2.556	1.00	1.07
ATOM		AL 333	3.547	4.419	0.756	1.00	0.24
MOTA		AL 333	3.562	4.741	-0.416	1.00	0.27
MOTA		AL 334	2.696	4.953	1.590	1.00	0.22
MOTA		AL 334	2.694	4.685	2.532	1.00	0.22
ATOM		AL 334	1.726	5.973 5.544	1.098	1.00	0.25 0.29
ATOM		AL 334 AL 334	1.127 0.812	6.420	0.310 2.244	1.00	0.29
ATOM ATOM		AL 334	1.410	6.823	3.048	1.00	0.30
ATOM	111 CG1 V		-0.151	7.491	1.735	1.00	0.40
ATOM	112 HG11 V		-0.343	7.329	0.685	1.00	1.10
ATOM	113 HG12 V		0.289	8.467	1.876	1.00	1.09
ATOM	114 HG13 V		-1.079	7.430	2.284	1.00	1.01
MOTA	115 CG2 V		-0.001	5.228	2.752	1.00	0.36
ATOM	116 HG21 V		-0.571	4.808	1.936	1.00	1.12
ATOM	117 HG22 V		-0.675	5.559	3.529	1.00	1.08 0.97
ATOM ATOM	118 HG23 V. 119 C V.	AL 334 AL 334	0.666 2.491	4.480 7.182	3.149 0.550	1.00	0.27
ATOM		AL 334	2.024	7.102	-0.332	1.00	0.32
ATOM		LU 335	3.661	7.443	1.067	1.00	0.31
MOTA		LU 335	4.021	6.874	1.779	1.00	0.35
MOTA		LU 335	4.450	8.608	0.573	1.00	0.38
MOTA		LU 335	3.776	9.380	0.231	1.00	0.40
ATOM		LU 335	5.316	9.155	1.710	1.00	0.41
MOTA	126 HB1 G		6.358	9.090	1.433	1.00	0.99
MOTA	127 HB2 G		5.144	8.574	2.604 1.971	1.00 1.00	1.01 1.26
MOTA MOTA	128 CG G 129 HG1 G	LU 335	4.951 3.896	10.617 10.691	2.188	1.00	1.99
MOTA	130 HG2 G		5.181	11.207	1.095	1.00	1.84
ATOM		LU 335	5.752	11.139	3.165	1.00	1.56
MOTA	132 OE1 G		5.139	11.659	4.082	1.00	2.26
MOTA	133 OE2 G		6.965	11.009	3.141	1.00	1.81
MOTA		LU 335	5.350	8.168	-0.584	1.00	0.41
MOTA		LU 335	5.396	8.797	-1.623	1.00	0.48
MOTA		SN 336	6.069	7.093	-0.411	1.00	0.41
ATOM ATOM		SN 336	6.019 6.970	6.603 6.612	0.436 -1.497	1.00	0.39 0.47
MOTA		SN 336	7.711	7.366	-1.712	1.00	0.53
MOTA		SN 336	7.665	5.327	-1.046	1.00	0.50
MOTA	141 HB1 A		7.812	4.680	-1.897	1.00	0.68
MOTA	142 HB2 A		7.052	4.824	-0.314	1.00	0.81
MOTA	143 CG A	SN 336	9.021	5.670	-0.429	1.00	0.81
MOTA	144 OD1 A		10.034	5.130	-0.825	1.00	1.73
MOTA	145 ND2 A		9.084	6.551	0.531	1.00	1.22
ATOM	146 HD21 A		8.266	6.986	0.851	1.00	1.80
MOTA MOTA	147 HD22 A 148 C A	SN 336 SN 336	9.949	6.777	0.933	1.00	1.52
MOTA		SN 336	6.156 6.262	6.334 7.036	-2.758 -3.744	1.00	0.45 0.53
MOTA		AL 337	5.347	5.312	-2.739	1.00	0.36
MOTA		'AL 337	5.277	4.755	-1.936	1.00	0.32
MOTA	152 CA V	'AL 337	4.534	4.992	-3.943	1.00	0.36
MOTA		'AL 337	5.192	4.703	-4.748	1.00	0.41
MOTA	154 CB V	'AL 337	3.585	3.838	-3.623	1.00	0.32

MOTA	155	HB	VAL	337	2.904	4.137	-2.841	1.00	0.33
MOTA	156	CG1	VAL	337	2.791	3.468	-4.877	1.00	0.36
MOTA	157	HG11	$\mathtt{VAL}$	337	2.519	4.368	-5.408	1.00	1.01
MOTA	158	HG12	VAL	337	1.898	2.933	-4.592	1.00	1.05
MOTA	159	HG13	VAL	337	3.398	2.843	-5.515	1.00	1.08
MOTA	160	CG2	VAL	337	4.398	2.626	-3.161	1.00	0.36
MOTA	161	HG21	VAL	337	5.411	2.933	-2.948	1.00	1.07
MOTA	162	HG22		337	4.404	1.879	-3.940	1.00	1.10
MOTA	163		VAL	337	3.952	2.213	-2.269	1.00	1.07
ATOM	164	C	VAL	337	3.721	6.228	-4.353	1.00	0.43
ATOM	165	ŏ	VAL	337	3.120	6.872	-3.517	1.00	0.44
	166			338	3.726	6.524	-5.631	1.00	0.51
ATOM		N	PRO						
ATOM	167	CA	PRO	338	2.973	7.700	-6.137	1.00	0.62
ATOM	168	HA	PRO	338	3.272	8.592	-5.611	1.00	0.65
MOTA	169	CB	PRO	338	3.393	7.792	-7.603	1.00	0.71
MOTA	170	HB1	PRO	338	4.218	8.477	-7.717	1.00	0.78
MOTA	171	HB2	PRO	338	2.556	8.101	-8.214	1.00	0.77
MOTA	172	CG	PRO	338	3.823	6.408	-7.962	1.00	0.64
MOTA	173	HG1	PRO	338	4.570	6.440	-8.740	1.00	0.71
MOTA	174	HG2	PRO	338	2.970	5.828	-8.287	1.00	0.63
MOTA	175	CD	PRO	338	4.415	5.810	-6.714	1.00	0.53
MOTA	176	HD2	PRO	338	4.209	4.749	-6.666	1.00	0.48
MOTA	177	HD1		338	5.476	5.997	-6.666	1.00	0.58
ATOM	178	С	PRO	338	1.460	7.465	-6.006	1.00	0.63
MOTA	179	Ö	PRO	338	0.977	6.393	-6.311	1.00	0.62
ATOM	180	Ŋ	PRO	339	0.758	8.476	-5.549	1.00	0.70
ATOM	181	CA	PRO	339	-0.712	8.361	-5.349	1.00	0.76
ATOM	182	HA							
			PRO	339	-0.965	7.452	-4.855	1.00	0.72
ATOM	183	CB	PRO	339	-1.066	9.568	-4.514	1.00	0.82
ATOM	184	HB1	PRO	339	-1.075	9.296	-3.470	1.00	0.77
MOTA	185	HB2	PRO	339	-2.027	9.967	-4.808	1.00	0.91
MOTA	186	CG	PRO	339	0.015	10.568	-4.772	1.00	0.87
MOTA	187	HG1	PRO	339	0.205	11.144	-3.880	1.00	0.89
MOTA	188	HG2	PRO	339	-0.278	11.224	-5.580	1.00	0.98
ATOM	189	CD	PRO	339	1.255	9.803	-5.154	1.00	0.78
MOTA	190	HD2	PRO	339	1.756	10.285	-5.982	1.00	0.85
AT©M	191	HD1	PRO	339	1.920	9.713	-4.309	1.00	0.76
ATOM	192	C	PRO	339	-1.443	8.438	-6.723	1.00	0.90
ATOM	193	0	PRO	339	-2.655	8.373	-6.780	1.00	1.13
MOTA	194	N	LEU	340	-0.728	8.587	-7.805	1.00	0.99
ATOM	195	HN	LEU	340	0.247	8.647	-7.749	1.00	1.13
ATOM	196	CA	LEU	340	-1.406	8.677	-9.129	1.00	1.11
ATOM	197	HA	LEU	340	-2.269	9.321	-9.045	1.00	1.47
MOTA	198	CB	LEU	340	-0.439	9.262	-10.161	1.00	1.35
MOTA	199	HB1		340	0.311		-10.409	1.00	1.21
ATOM	200	HB2		340	0.039	10.140	-9.749	1.00	1.73
ATOM	201	CG	LEU	340	-1.213		-11.424		
ATOM	202	HG	LEU	340	-1.213		-11.424 $-11.842$	1.00	1.45
MOTA	203	CD1						1.00	1.29
ATOM		HD11		340	-2.293		-11.071	1.00	1.81
				340	-1.936		-10.279	1.00	2.38
MOTA		HD12		340	-3.184		-10.744	1.00	1.87
ATOM		HD13		340	-2.521		-11.942	1.00	2.04
ATOM	207	CD2		340	-0.251		-12.447	1.00	1.78
ATOM		HD21		340	0.768		-12.147	1.00	1.70
MOTA	209	HD22	LEU	340	-0.408	11.320	-12.500	1.00	2.32
MOTA		HD23		340	-0.433	9.814	-13.417	1.00	2.30
MOTA	211	C	LEU	340	-1.855	7.287	-9.585	1.00	0.73
MOTA	212	0	LEU	340	-2.990	7.089	-9.972	1.00	0.98
MOTA	213	N	ARG	341	-0.975	6.325	-9.555	1.00	0.40
MOTA	214	HN	ARG	341	-0.062	6.505	-9.247	1.00	0.41
MOTA	215	CA	ARG	341	-1.356	4.953	-10.000	1.00	0.68
MOTA	216	HA	ARG	341	-2.323		-10.480	1.00	0.99
MOTA	217	CB	ARG	341	-0.311		-10.993	1.00	1.12
MOTA	218	HB1		341	-0.378		-11.054	1.00	1.46
MOTA	219	HB2		341	0.676		-10.654	1.00	1.51
MOTA	220	CG	ARG	341	-0.566		-12.380	1.00	1.89
MOTA	221	HG1		341	-1.485		-12.782	1.00	2.12
ATOM	222	HG2		341	0.253		-13.038	1.00	2.12
ATOM	223	CD	ARG	341	-0.679		-12.269		
ATOM	224	HD1		341	0.021			1.00	2.83
ATOM	225	HD2		341	-1.684	0.313	-11.526	1.00	3.07
ATOM	226	NE	ARG	341	-1.684 -0.375		-11.966	1.00	2.89
MOTA	227	HE	ARG	341	-1.083		-13.589	1.00	3.77
ATOM	228	CZ	ARG	341	0.832		-14.260	1.00	3.89
MOTA	229	NH1		341			-13.851	1.00	4.65
ATOM		HH11			1.861		-13.266	1.00	5.32
MOTA	221	TITIO	AKG	341	1.726		-12.616	1.00	5.28
TION	Z31	HH12	AKG	341	2.785	7.382	-13.469	1.00	6.08

ATOM	232	NH2	ARC	341	1.011	8 584	-14.701	1.00	5.18
MOTA		HH21		341	0.223		-15.149	1.00	5.01
MOTA	234	HH22	ARG	341	1.935	8.909	-14.903	1.00	5.96
MOTA	235	С	ARG	341	-1.421	4.033	-8.790	1.00	0.54
ATOM	236	ō	ARG	341	-1.148	2.852	-8.872	1.00	0.50
MOTA	237	N	TRP	342	-1.781	4.573	-7.662	1.00	0.53
MOTA	238	HN	TRP	342	-1.991	5.532	-7.631	1.00	0.61
MOTA	239	CA	TRP	342	-1.866	3.740	-6.426	1.00	0.42
ATOM	240	HA	TRP	342	-0.870	3.445	-6.127	1.00	0.43
MOTA	241	CB	TRP	342	-2.513	4.543	-5.295	1.00	0.43
MOTA	242	HB1	TRP	342	-3.557	4.705	-5.518	1.00	0.47
ATOM	243	HB2	TRP	342	-2.011	5.494	-5.194	1.00	0.50
ATOM	244	CG	TRP	342	-2.387	3.771	-4.022	1.00	0.34
ATOM	245	CD1		342	-3.270	2.845	-3.583	1.00	0.35
MOTA	246	HD1	TRP	342	-4.177	2.553	-4.091	1.00	0.42
MOTA	247	CD2	TRP	342	-1.330	3.834	-3.021	1.00	0.30
ATOM	248	NE1	ጥጽኮ	342	-2.819	2.332	-2.380	1.00	0.31
ATOM	249	HE1		342	-3.276	1.644	-1.853	1.00	0.35
ATOM	250	CE2		342	-1.628	2.911	-1.991	1.00	0.28
MOTA	251	CE3	TRP	342	-0.153	4.595	-2.910	1.00	0.34
MOTA	252	HE3	TRP	342	0.100	5.308	-3.681	1.00	0.39
ATOM	253			342	0.785	2.747	-0.889	1.00	0.31
MOTA	254	HZ2		342	-1.030	2.032	-0.116	1.00	0.35
ATOM	255	CZ3	TRP	342	0.695	4.435	-1.803	1.00	0.37
ATOM	256	HZ3	TRP	342	1.595	5.026	-1.727	1.00	0.44
ATOM	257	CH2		342	0.380	3.513	-0.795	1.00	0.35
ATOM	258			342	1.036	3.397	0.055	1.00	0.42
ATOM	259	С	TRP	342	-2.701	2.485	-6.700	1.00	0.35
MOTA	260	0	TRP	342	-2.269	1.378	-6.444	1.00	0.34
ATOM	261	N	LYS	343	-3.892	2.646	-7.223	1.00	0.36
ATOM	262	HN	LYS	343	-4.218				
						3.548	-7.425	1.00	0.41
MOTA	263	CA	LYS	343	-4.755	1.458	-7.518	1.00	0.34
MOTA	264	HA	LYS	343	-5.115	1.032	-6.589	1.00	0.35
ATOM	265	CB	LYS	343	-5.946	1.892	-8.375	1.00	0.40
ATOM	266	HB1		343	-5.592	2.240	-9.334	1.00	0.41
ATOM	267								
		HB2		343	-6.478	2.689	-7.875	1.00	0.47
MOTA	268	CG	LYS	343	-6.885	0.702	-8.583	1.00	0.43
MOTA	269	HG1	LYS	343	-7.307	0.406	-7.634	1.00	0.48
MOTA	270	HG2	LYS	343	-6.330	-0.124	-9.004	1.00	0.40
MOTA	271	CD	LYS	343	-8.012	1.099	-9.537	1.00	0.50
	272								
MOTA		HD1		343	-7.664		-10.557	1.00	0.70
ATOM	273	HD2	LYS	343	-8.315	2.116	-9.333	1.00	0.82
MOTA	274	CE	LYS	343	-9.203	0.161	-9.337	1.00	0.87
MOTA	275	HE1	LVS	343	-9.772	0.479	-8.476	1.00	1.44
MOTA	276	HE2		343	-8.846	-0.846	-9.181	1.00	1.38
MOTA	277	NZ	LYS	343	-10.073		-10.547	1.00	1.58
ATOM	278	HZ1	LYS	343	-10.202	1.183	-10.852	1.00	2.04
MOTA	279	HZ2	LYS	343	-10.999	-0.221	-10.321	1.00	2.03
MOTA	280	HZ3		343	-9.625		-11.313	1.00	2.15
ATOM	281	C	LYS	343	-3.939	0.407			
							-8.273	1.00	0.34
MOTA	282	0	LYS	343	-3.994	-0.768	-7.971	1.00	0.36
MOTA	283	N	GLU	344	-3.160	0.822	-9.238	1.00	0.38
ATOM	284	HN	GLU	344	-3.111	1.776	-9.456	1.00	0.40
ATOM	285	CA	GLU	344	-2.324	-0.160	-9.981	1.00	0.44
MOTA	286	HA	GLU	344	-2.959		-10.469		
								1.00	0.47
ATOM	287	CB	GLU	344	-1.472		-11.021	1.00	0.53
MOTA	288	HB1		344	-0.656	-0.066	-11.329	1.00	0.90
MOTA	289	HB2	GLU	344	-1.077	1.478	-10.588	1.00	0.68
MOTA	290	CG	GLU	344	-2.333		-12.237	1.00	1.19
MOTA	291	HG1		344	-2.676			1.00	
ATOM	292						-12.157	1.00	1.51
		HG2		344	-3.184		-12.276	1.00	1.62
MOTA	293	CD	GLU	344	-1.502		-13.512	1.00	1.27
MOTA	294	OE1	GLU	344	-0.287		-13.412	1.00	1.38
MOTA	295	OE2		344	-2.095		-14.567	1.00	1.96
MOTA	296								
		C	GLU	344	-1.418	-0.861	-8.972	1.00	0.42
ATOM	297	0	GLU	344	-1.350	-2.073	-8.911	1.00	0.43
MOTA	298	N	PHE	345	-0.746	-0.096	-8.155	1.00	0.40
MOTA	299	HN	PHE	345	-0.842	0.878	-8.209	1.00	0.40
ATOM	300	CA	PHE	345					
					0.133	-0.696	-7.117	1.00	0.39
ATOM	301	HA	PHE	345	0.911	-1.281	-7.586	1.00	0.41
MOTA	302	CB	PHE	345	0.754	0.436	-6.287	1.00	0.38
MOTA	303	HB1		345	-0.028	1.101	-5.953	1.00	0.40
MOTA	304	HB2		345	1.450	0.987	-6.902	1.00	0.41
ATOM	305	CG	PHE	345	1.485				
MOTA	306					-0.117	-5.083	1.00	0.36
		CD1		345	1.435	0.573	-3.867	1.00	1.30
ATOM	307	HD1		345	0.870	1.491	-3.790	1.00	2.21
MOTA	308	CD2	PHE	345	2.217	-1.306	-5.182	1.00	1.22
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MOTA	309		PHE	345	2.255	-1.842	-6.117	1.00	2.14
MOTA	310	CE1	PHE	345	2.115	0.077	-2.750	1.00	1.31
MOTA	311		PHE	345	2.075	0.612	-1.812	1.00	2.23
MOTA	312	CE2	PHE	345	2.896	-1.803	-4.064	1.00	1.21
MOTA	313	HE2	PHE	345	3.461	-2.718	-4.141	1.00	2.12
MOTA	314	CZ	PHE	345	2.846	-1.112	-2.848	1.00	0.37
ATOM	315	HZ	PHE	345	3.372	-1.496	-1.986	1.00	0.39
ATOM	316	C	PHE	345	-0.730	-1.594	-6.232	1.00	0.37
ATOM	317	Õ	PHE	345	-0.730	-2.595	-5.709	1.00	0.37
MOTA					-1.977	-2.393	-6.083	1.00	0.37
	318	N	VAL	346					
MOTA	319	HN	VAL	346	-2.313	-0.438	-6.529	1.00	0.39
ATOM	320	CA	VAL	346	-2.896	-2.068	-5.259	1.00	0.40
MOTA	321	HA	VAL	346	-2.407	-2.356	-4.339	1.00	0.40
MOTA	322	CB	VAL	346	-4.150	-1.251	-4.944	1.00	0.52
ATOM	323	$^{ m HB}$	VAL	346	-4.658	-1.002	-5.865	1.00	1.31
MOTA	324		VAL	346	-5.084	-2.064	-4.054	1.00	1.22
ATOM	325	HG11	VAL	346	-4.578	-2.309	-3.134	1.00	1.73
ATOM	326	HG12	VAL	346	-5.366	-2.972	-4.565	1.00	1.84
MOTA	327			346	-5.968	-1.482	-3.837	1.00	1.77
ATOM	328		VAL	346	-3.751	0.034	-4.217	1.00	0.88
ATOM		HG21		346	-3.741	0.856	-4.917	1.00	1.44
ATOM		HG22		346	-2.767	-0.085	-3.788	1.00	1.55
ATOM	331	HG23		346	-4.463	0.240	-3.431	1.00	1.48
ATOM	332		VAL						
		C		346	-3.276	-3.317	-6.055	1.00	0.37
ATOM	333	0	VAL	346	-3.377	-4.406	-5.519	1.00	0.37
ATOM	334	N	LYS	347	-3.467	-3.171	-7.341	1.00	0.38
ATOM	335	HN	LYS	347	-3.363	-2.289	-7.756	1.00	0.39
MOTA	336	CA	LYS	347	-3.817	-4.351	-8.176	1.00	0.39
MOTA	337	HA	LYS	347	-4.726	-4.803	-7.806	1.00	0.40
AŒOM .	338	CB	LYS	347	-4.009	-3.915	-9.631	1.00	0.43
ATOM	339	HB1	LYS	347	-3.428	-4.554	-10.278	1.00	0.81
ATOM	340	HB2	LYS	347	-3.681	-2.892	-9.745	1.00	0.77
ATOM	341	CG	LYS	347	-5.489			1.00	0.92
ATOM	342	HG1	LYS	347	-6.078	-3.422	-9.332	1.00	1.27
ATOM	343		LYS	347	-5.803	-5.054	-9.942	1.00	1.24
ATOM	344	CD	LYS	347	-5.688		-11.440	1.00	1.11
ATOM	345		LYS	347	-5.098		-12.117	1.00	1.38
ATOM	346		LYS	347	-5.374		-11.504	1.00	1.25
ATOM	347	CE	LYS	347	-7.166		-11.821	1.00	1.99
ATOM	348		LYS	347	-7.728			1.00	
ATOM	349			347			-11.309		2.39
ATOM		NZ	LYS		-7.540		-11.536	1.00	2.52
	350		LYS	347	-7.312		-13.294	1.00	2.35
ATOM	351		LYS	347	-8.189		-13.496	1.00	2.93
ATOM	352		LYS	347	-7.350		-13.753	1.00	2.57
ATOM	353	_	LYS	347	-6.501	-2.915	-13.662	1.00	2.47
ATOM	354	С	LYS	347	-2.671	-5.354	-8.086	1.00	0.39
MOTA	355	0	LYS	347	-2.873	-6.530	-7.854	1.00	0.41
ATOM	356	N	ARG	348	-1.461	-4.890	-8.246	1.00	0.39
MOTA	357	HN	ARG	348	-1.322	-3.935	-8.416	1.00	0.39
MOTA	358	CA	ARG	348	-0.295	-5.806	-8.146	1.00	0.42
MOTA	359	HA	ARG	348	-0.412	-6.624	-8.842	1.00	0.47
MOTA	360	CB	ARG	348	0.990	-5.037	-8.462	1.00	0.45
MOTA	361		ARG	348	1.843	-5.678	-8.300	1.00	0.75
MOTA	362		ARG	348	1.061	-4.173	-7.816	1.00	0.95
ATOM	363	CG	ARG	348	0.968	-4.581	-9.923	1.00	1.12
ATOM	364		ARG	348	1.496		-10.016	1.00	1.84
MOTA	365		ARG	348	-0.055		-10.244	1.00	1.77
ATOM	366	CD	ARG	348	1.649		-10.799	1.00	
ATOM	367		ARG	348	1.059				1.28
MOTA	368		ARG	348			-10.797	1.00	1.54
MOTA	369	NE			2.634		-10.409	1.00	1.76
			ARG	348	1.765		-12.193	1.00	2.08
MOTA	370	HE	ARG	348	1.642		-12.374	1.00	2.58
MOTA	371	CZ	ARG	348	2.032		-13.172	1.00	2.53
ATOM	372		ARG	348	1.143		-13.548	1.00	3.15
MOTA		HH11		348	0.257		-13.086	1.00	3.43
ATOM		HH12		348	1.347		-14.298	1.00	3.63
MOTA	375		ARG	348	3.188		-13.775	1.00	2.91
MOTA		HH21		348	3.869	-5.210	-13.487	1.00	3.03
MOTA	377		ARG	348	3.392		-14.525	1.00	3.41
MOTA	378	С	ARG	348	-0.231	-6.348	-6.719	1.00	0.40
MOTA	379	0	ARG	348	0.253	-7.435	-6.474	1.00	0.43
MOTA	380	N	LEU	349	-0.732	-5.596	-5.774	1.00	0.36
MOTA	381	HN	LEU	349	-1.124	-4.726	-5.997	1.00	0.35
ATOM	382	CA	LEU	349	-0.718	-6.060	-4.360	1.00	0.37
MOTA	383	HA	LEU	349	0.302	-6.157	-4.020	1.00	0.39
MOTA	384	CB	LEU	349	-1.454	-5.043	-3.486	1.00	0.36
ATOM	385		LEU	349	-2.389	-5.464	-3.149	1.00	0.48
					2.005		3.143	1.00	0.40

ATOM	386	HB2	LEU	349	-1.649	-4.149	-4.062	1.00	0.41
MOTA	387	CG	LEU	349	-0.589	-4.692	-2.275	1.00	0.40
MOTA	388	HG	LEU	349	0.051	-5.529	-2.036	1.00	0.65
MOTA	389		LEU	349	0.270	-3.469	-2.600	1.00	0.52
MOTA		HD11		349	1.268	-3.789	-2.859	1.00	1.02
MOTA		HD12		349	0.313	-2.820	-1.737	1.00	1.18
MOTA MOTA	392 393	HD13	LEU	349 349	-0.165 -1.491	-2.934 -4.378	-3.431 -1.081	1.00	1.30
ATOM		HD21		349	-1.483	-3.315	-0.894	1.00	1.15
ATOM	395	HD22		349	-1.127	-4.901	-0.208	1.00	1.15
MOTA	396		LEU	349	-2.500	-4.698	-1.298	1.00	1.11
MOTA	397	С	LEU	349	-1.417	-7.418	-4.274	1.00	0.38
ATOM	398	0	LEU	349	-0.853	-8.389	-3.811	1.00	0.40
ATOM	399	N	GLY	350	-2.637	-7.499	-4.731	1.00	0.38
MOTA MOTA	400 401	HN CA	GLY GLY	350 350	-3.073 -3.358	-6.706 -8.804	-5.113 -4.686	1.00 1.00	0.39 $0.41$
MOTA	402	HA1		350	-2.725	-9.545	-4.220	1.00	0.49
MOTA	403	HA2		350	-3.593	-9.117	-5.693	1.00	0.46
MOTA	404	С	GLY	350	-4.653	-8.672	-3.880	1.00	0.32
MOTA	405	0	GLY	350	-5.238	-9.655	-3.471	1.00	0.32
ATOM	406	N	LEU	351	-5.114	-7.473	-3.650	1.00	0.31
ATOM ATOM	407 408	HN CA	LEU LEU	351 351	-4.637 -6.375	-6.688	-3.988	1.00	0.35
ATOM	409	HA	LEU	351	-6.460	-7.304 -8.100	-2.876 -2.151	1.00	0.28
ATOM	410	CB	LEU	351	-6.359	-5.956	-2.153	1.00	0.34
MOTA	411		LEU	351	-6.954	-5.244	-2.705	1.00	0.78
MOTA	412	HB2	LEU	351	-5.342	-5.598	-2.082	1.00	0.74
MOTA	413	CG	LEU	351	-6.943	-6.124	-0.749	1.00	0.69
ATOM	414	HG	LEU	351	-7.915	-6.590	-0.818	1.00	1.53
MOTA MOTA	415	HD11	LEU	351 351	-6.014 -5.298	-7.004 7.401	0.090 -0.556	1.00	1.03
ATOM	417			351	-6.598	-7.491 -7.751	0.608	$1.00 \\ 1.00$	1.65 1.55
MOTA	418	HD13		351	-5.492	-6.393	0.811	1.00	1.45
ATOM	419	CD2	LEU	351	-7.078	-4.751	-0.087	1.00	1.36
MOTA	420	HD21	LEU	351	-7.424	-4.034	-0.816	1.00	1.71
MOTA		HD22		351	-6.118	-4.440	0.297	1.00	1.92
MOTA MOTA	422 423	HD23 C	LEU LEU	351 351	-7.788 -7.566	-4.811	0.724	1.00	1.96
ATOM	424	o	LEU	351	-7.434	-7.358 -7.119	-3.833 -5.017	1.00 1.00	0.28
ATOM	425	Ň	SER	352	-8.730	-7.674	-3.333	1.00	0.32
MOŢA	426	HN	SER	352	-8.815	-7.866	-2.376	1.00	0.35
MOTA	427	CA	SER	352	-9.928	-7.746	-4.218	1.00	0.39
MOTA	428	HA	SER	352	-9.812	-8.564	-4.914	1.00	0.42
MOTA MOTA	429 430	CB HB1	SER SER	352 352	-11.176 -11.572	-7.977 -7.033	-3.366 -3.044	1.00	0.50
ATOM	431	HB2	SER	352	-10.921	-7.022 -8.566	-3.044	$1.00 \\ 1.00$	0.91 0.98
MOTA	432	OG	SER	352	-12.147	-8.672	-4.136	1.00	1.21
ATOM	433	HG	SER	352	-12.309	-9.520	-3.715	1.00	1.44
MOTA	434	C	SER	352	-10.076	-6.435	-4.993	1.00	0.38
MOTA	435	0	SER	352	-10.150	-5.367	-4.418	1.00	0.36
MOTA MOTA	436 437	N HN	ASP ASP	353 353	-10.120 -10.060	-6.507	-6.296	1.00	0.41
ATOM	438	CA	ASP	353	-10.060	-7.379 -5.266	-6.740 -7.108	$1.00 \\ 1.00$	0.44
ATOM	439	HA	ASP	353	-9.387	-4.650	-6.984	1.00	0.41
MOTA	440	CB	ASP	353	-10.422	-5.639	-8.584	1.00	0.49
ATOM	441		ASP	353	-11.358	-5.249	-8.956	1.00	1.06
MOTA MOTA	442 443		ASP	353	-10.413	-6.714	-8.686	1.00	1.01
ATOM	444	CG OD1	ASP ASP	353 353	-9.267	-5.039	-9.388	1.00	1.39
ATOM	445		ASP	353	-9.539 -8.130	-5.241	-10.384 -8.995	$1.00 \\ 1.00$	2.17 2.10
MOTA	446	C	ASP	353	-11.501	-4.493	-6.643	1.00	0.43
MOTA	447	0	ASP	353	-11.497	-3.280	-6.574	1.00	0.40
MOTA	448	N	HIS	354	-12.558	-5.187	-6.319	1.00	0.50
MOTA	449	HN	HIS	354	-12.540	-6.165	-6.379	1.00	0.55
MOTA MOTA	450	CA	HIS	354	-13.790	-4.490	-5.856	1.00	0.56
ATOM	451 452	HA CB	HIS HIS	354 354	-14.088 -14.914	-3.757 -5.511	-6.591	1.00	0.58
ATOM	453		HIS	354	-14.914 -15.268	-5.511 -5.468	-5.663 -4.644	1.00 1.00	0.68 1.10
ATOM	454		HIS	354	-14.539	-6.502	-5.873	1.00	1.33
MOTA	455	CG	HIS	354	-16.047	-5.194	-6.600	1.00	1.29
ATOM	456		HIS	354	-15.862	-5.075	-7.969	1.00	2.24
MOTA	457		HIS	354	-15.015	-5.182	-8.450	1.00	2.68
MOTA MOTA	458 459		HIS HIS	354 354	-17.382	-4.965	-6.381	1.00	2.16
ATOM	460		HIS	354	-17.866 -17.057	-4.981 -4.787	-5.416 -8.516	1.00 1.00	2.62
MOTA	461		HIS	354	-17.219	-4.638	-9.573	1.00	3.92
MOTA	462		HIS	354	-18.019	-4.708	-7.592	1.00	3.02

MOTA	463 C HI		-13.502	-3.790	-4.528	1.00	0.49
MOTA	464 O HI		-13.852	-2.643	-4.332	1.00	0.49
MOTA	465 N GL		-12.860	-4.467	-3.616	1.00	0.49
MOTA	466 HN GL		-12.581	-5.389	-3.794	1.00	0.50
ATOM	467 CA GLI		-12.546	-3.832	-2.306	1.00	0.49
ATOM	468 HA GLI		-13.465	-3.596	-1.789	1.00	0.56
ATOM	469 CB GLI		-11.713	-4.794	-1.456	1.00	0.55
ATOM	470 HB1 GL		-10.802	-5.041	-1.980	1.00	0.96
ATOM	471 HB2 GL		-12.280	-5.695	-1.273	1.00	0.95
MOTA	472 CG GLI		-11.366	-4.128	-0.123	1.00	1.01
MOTA	473 HG1 GL		-12.239	-3.628	0.267	1.00	1.63
MOTA	474 HG2 GL		-10.575	-3.408	-0.276	1.00	1.68
MOTA	475 CD GL		-10.904	-5.192	0.873	1.00	1.40
MOTA MOTA	476 OE1 GLV		-9.849	-5.010	1.458	1.00	2.07
MOTA	477 OE2 GLI 478 C GLI		-11.613	-6.172	1.033	1.00	1.91
ATOM	478 C GL		-11.753 -11.879	-2.548 -1.581	-2.551	1.00	0.40
ATOM	480 N IL		-10.942	-2.533	-1.828 -3.574	1.00	0.43
MOTA	481 HN IL		-10.861	-3.324	-3.574	1.00	0.33
ATOM	482 CA ILI		-10.143	-1.313	-3.876	1.00	
ATOM	483 HA ILI		-9.520	-1.071	-3.028	1.00	0.30 0.35
ATOM	484 CB ILI		-9.258	-1.577	-5.023	1.00	0.33
ATOM	485 HB IL		-9.875	-1.872	-5.933	1.00	0.36
ATOM	486 CG1 ILI		-8.270	-2.698	-4.766	1.00	0.39
ATOM	487 HG11 ILI		-8.815	-3.601	-4.537	1.00	0.38
ATOM	488 HG12 IL		-7.674	-2.411	-3.913	1.00	0.38
ATOM	489 CG2 ILI		-8.484	-0.305	-5.457	1.00	0.39
MOTA	490 HG21 IL		-8.663	0.450	-4.706	1.00	1.08
ATOM	491 HG22 ILI		-8.816	0.057	-6.419	1.00	1.06
MOTA	492 HG23 ILI		-7.428	-0.527	-5.501	1.00	1.06
ATOM	493 CD1 ILI		-7.357	-2.947	-5.967	1.00	0.47
ATOM	494 HD11 IL		-6.572	-2.207	-5.981	1.00	1.16
A <b>T</b> OM	495 HD12 ILE		-7.934	-2.878	-6.877	1.00	1.16
MOTA	496 HD13 ILI		-6.922	-3.933	-5.889	1.00	1.07
MOTA	497 C ILE		-11.090	-0.147	-4.167	1.00	0.31
AT⊕M	498 O ILI		-10.833	0.981	-3.799	1.00	0.34
MOTA	499 N ASI		-12.187	-0.412	-4.824	1.00	0.34
ATOM	500 HN ASI		-12.378	-1.330	-5.111	1.00	0.37
MOTA	501 CA ASI		-13.151	0.681	-5.134	1.00	0.40
MÖTA	502 HA ASI		-12.619	1.522	-5.554	1.00	0.43
ATOM ATOM	503 CB ASI		-14.187	0.178	-6.142	1.00	0.48
MOTA	504 HB1 ASE 505 HB2 ASE		-15.158	0.575	-5.888	1.00	0.96
MOTA	505 HB2 ASI 506 CG ASI		-14.220	-0.901	-6.115	1.00	0.95
MOTA	500 CG ASI		-13.801	0.642	-7.548	1.00	1.24
ATOM	508 OD2 ASE		-13.679 -13.635	-0.205	-8.417		
ATOM	509 C ASE		-13.858	1.837 1.113	-7.732 -3.848	1.00	2.06
ATOM	510 O ASI		-14.333	2.226	-3.733	1.00	$0.41 \\ 0.45$
ATOM	511 N ARG		-13.932	0.241	-2.880	1.00	0.43
MOTA	512 HN ARG		-13.543	-0.651	-2.880	1.00	0.43
MOTA	513 CA ARG		-14.609	0.599	-1.601	1.00	0.49
MOTA	514 HA ARG		-15.482	1.186	-1.816	1.00	0.50
MOTA	515 CB ARG		-15.019	-0.677	-0.863	1.00	0.57
MOTA	516 HB1 ARG	358	-15.605	-0.417	0.006	1.00	0.92
ATOM	517 HB2 ARG	358	-14.134	-1.214	-0.554	1.00	0.75
MOTA	518 CG ARG		-15.854	-1.561	-1.791	1.00	1.10
ATOM	519 HG1 ARG		-15.244	-1.895	-2.616	1.00	1.46
MOTA	520 HG2 ARG		-16.693	-0.995	-2.168	1.00	1.66
MOTA	521 CD ARG		-16.365	-2.777	-1.015	1.00	1.30
MOTA	522 HD1 ARG		-15.551	-3.214	-0.455	1.00	1.75
MOTA	523 HD2 ARG		-16.759	-3.506	-1.707	1.00	1.56
ATOM ATOM	524 NE ARG 525 HE ARG		-17.441	-2.352	-0.076	1.00	1.98
ATOM			-17.515	-1.412	0.193	1.00	2.56
ATOM	526 CZ ARG 527 NH1 ARG		-18.286	-3.232	0.390	1.00	2.40
MOTA	527 NHI ARG		-18.371	-3.438	1.676	1.00	3.04
ATOM	529 HH12 ARG	358 358	-17.790 -19.019	-2.922	2.305	1.00	3.32
ATOM	530 NH2 ARG		-19.018 -19.044	-4.112	2.032	1.00	3.55
ATOM	531 HH21 ARG	358	-19.044 -18.979	-3.905	-0.431	1.00	2.82
ATOM	532 HH22 ARG		-18.979 -19.691	-3.747	-1.416	1.00	3.00
MOTA	533 C ARG		-19.691	-4.579 $1.412$	-0.075	1.00	3.31
MOTA	534 O ARG		-13.000 -14.079	2.100	-0.720 0.190	1.00	0.50 0.56
MOTA	535 N LEU		-12.388	1.337	-0.979	1.00	0.36
MOTA	536 HN LEU		-12.077	0.777	-1.715	1.00	0.45
ATOM	537 CA LEU		-11.412	2.104	-0.151	1.00	0.54
MOTA	538 HA LEU	359	-11.525	1.824	0.886	1.00	0.61
MOTA	539 CB LEU	359	-9.978	1.800	-0.608	1.00	0.56
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ATOM	540	HB1	ד זיבו ד	359	-9.284	2.152	0.141	1.00	0.78
ATOM	541	HB2		359	-9.786	2.309	-1.541	1.00	0.86
ATOM	542	CG	LEU	359	-9.784	0.291	-0.806	1.00	0.58
ATOM	543	HG	LEU	359	-10.359	-0.035	-1.658	1.00	1.08
ATOM	544	CD1		359	-8.304	-0.003	-1.054	1.00	0.81
MOTA	545	HD11	LEU	359	-7.991	0.471	-1.972	1.00	1.55
MOTA		HD12		359	-8.157	-1.070	-1.131	1.00	1.29
MOTA		HD13		359	-7.719	0.382	-0.232	1.00	1.26
ATOM	548	CD2		359	-10.240	-0.469	0.443	1.00	0.98
MOTA		HD21 HD22		359	-11.287 -10.091	-0.717 0.150	0.351 1.315	1.00 1.00	$1.62 \\ 1.46$
MOTA MOTA			LEU	359 359	-9.662	-1.376	0.542	1.00	1.49
ATOM	552	C	LEU	359	-11.684	3.601	-0.305	1.00	0.58
ATOM	553	ŏ	LEU	359	-11.683	4.343	0.657	1.00	0.67
ATOM	554	Ň	GLU	360	-11.916	4.050	-1.507	1.00	0.59
MOTA	555	HN	GLU	360	-11.913	3.435	-2.270	1.00	0.56
MOTA	556	CA	GLU	360	-12.188	5.499	-1.720	1.00	0.72
MOTA	557	HA	GLU	360	-11.354	6.079	-1.352	1.00	0.78
MOTA	558	CB	GLU	360	-12.379	5.770	-3.213	1.00	0.81
MOTA	559	HB1		360	-13.419	5.640	-3.473	1.00	1.05
MOTA	560	HB2		360 360	-11.775 -11.953	5.080 7.205	-3.784 -3.530	1.00 1.00	0.96 1.67
ATOM ATOM	561 562	CG HG1	GLU	360	-11.953	7.414	-3.050	1.00	2.26
MOTA	563	HG2		360	-12.703	7.892	-3.164	1.00	2.21
ATOM	564	CD	GLU	360	-11.802	7.371	-5.043	1.00	1.94
MOTA	565		GLU	360	-12.814	7.358	-5.724	1.00	2.33
MOTA	566	OE2	GLU	360	-10.677	7.508	-5.494	1.00	2.49
MOTA	567	С	GLU	360	-13.456	5.894	-0.962	1.00	0.76
MOTA	568	0	GLU	360	-13.577	6.997	-0.466	1.00	0.86
ATOM	569	N	LEU	361	-14.403	5.001	-0.868	1.00	0.74
ATOM	570	HN	LEU	361	-14.285	4.117	-1.274	1.00	0.69
ATOM ATOM	571 572	CA	LEU LEU	361 361	-15.662 -16.056	5.325 6.264	-0.141 -0.503	1.00	0.86 0.95
ATOM	573	HA CB	LEU	361	-16.688	4.215	-0.382	1.00	0.96
ATOM	574	HB1		361	-16.739	3.577	0.488	1.00	1.36
ATOM	575	HB2		361	-16.391	3.631	-1.241	1.00	1.11
ATOM	576	CG	LEU	361	-18.063	4.834	-0.636	1.00	1.71
ATOM	577	HG	LEU	361	-18.061	5.863	-0.306	1.00	2.43
ATOM	578		LEU	361	-18.381	4.780	-2.131	1.00	2.03
MOTA	579	HD11		361	-17.459	4.767	-2.695	1.00	2.51
MOTA MOTA	580	HD12 HD13		361 361	-18.959	5.649 3.887	-2.408 -2.347	1.00	2.43 2.25
ATOM	582		LEU	361	-18.948 -19.125	4.050	0.137	1.00	2.23
MOTA	583	HD21		361	-18.693	3.135	0.515	1.00	2.74
ATOM		HD22		361	-19.949	3.814	-0.520	1.00	2.84
ATOM	585	HD23	LEU	361	-19.484	4.646	0.963	1.00	2.65
ATOM	586	С	LEU	361	-15.371	5.437	1.357	1.00	0.89
ATOM	587	0	LEU	361	-15.986	6.211	2.063	1.00	1.03
ATOM	588	N	GLN	362	-14.435	4.669	1.848	1.00	0.83
ATOM ATOM	589 590	HN	GLN	362 362	-13.950 -14.104	4.052 4.732	1.261	1.00	0.76
MOTA	591	CA HA	GLN GLN	362	-14.104	4.732	3.300 3.877	1.00	0.95 1.11
MOTA	592	CB	GLN	362	-12.900	3.834	3.589	1.00	0.97
MOTA	593		GLN	362	-12.015	4.442	3.701	1.00	1.37
MOTA	594		GLN	362	-12.761	3.143	2.769	1.00	1.26
MOTA	595	CG	GLN	362	-13.144	3.051	4.881	1.00	1.37
ATOM	596		GLN	362	-14.040	2.459	4.779	1.00	1.85
ATOM	597		GLN	362	-13.260	3.743	5.703	1.00	2.00
MOTA MOTA	598 599	CD OF1	GLN GLN	362 362	-11.954 -10.989	2.129 2.129	5.153 4.415	1.00	$\frac{1.42}{1.39}$
ATOM	600		GLN	362	-11.983	1.336	6.190	1.00	2.20
ATOM		HE21		362	-12.761	1.336	6.785	1.00	2.72
ATOM				362	-11.226	0.742	6.373	1.00	2.46
MOTA	603	С	GLN	362	-13.768	6.174	3.686	1.00	1.04
ATOM	604	0	GLN	362	-14.293	6.709	4.642	1.00	1.30
ATOM	605	N	ASN	363	-12.896	6.809	2.950	1.00	1.02
ATOM	606	HN	ASN	363	-12.483	6.360	2.183	1.00	1.03
MOTA MOTA	607 608	CA HA	ASN	363 363	-12.529	8.214	3.279	1.00	1.24
ATOM	609	CB	ASN ASN	363 363	-13.404 -11.459	8.741 8.218	3.631 4.373	1.00	1.45 1.35
ATOM	610		ASN	363	-10.738	8.218	$\frac{4.373}{4.170}$	1.00	1.46
ATOM	611		ASN	363	-10.962	7.259	4.392	1.00	1.49
ATOM	612	CG	ASN	363	-12.118	8.479	5.728	1.00	2.07
ATOM	613		ASN	363	-12.924	9.378	5.862	1.00	2.60
MOTA MOTA	614		ASN	363	-11.809	7.724	6.747	1.00	2.76
ATOM MOTA		HD21 HD22		363 363	-11.159	6.999	6.640	1.00	2.99
011	010	111122	UDIA	202	-12.227	7.883	7.619	1.00	3.34

ATOM	617	С	ASN	363	-	11.987	8.908	2.028	1.00	1.40
ATOM	618	0	ASN	363	_	10.813	9.206	1.930	1.00	2.25
MOTA	619		GLY	364		12.834	9.166	1.069	1.00	1.09
MOTA	620		GLY	364		13.777	8.917	1.169	1.00	1.35
MOTA	621	CA	GLY	364	-	12.371	9.840	-0.177	1.00	1.25
ATOM	622	HA1	GLY	364	_	13.191	9.907	-0.876	1.00	1.54
MOTA	623	HA2	GLY.	364	_	11.569	9.264	-0.618	1.00	1.26
ATOM	624		GLY	364		11.868	11.249	0.148	1.00	1.27
						11.155	11.856	-0.626	1.00	1.55
ATOM	625		GLY	364						
MOTA	626		ARG	365		12.234	11.780	1.286	1.00	1.27
MOTA	627	HN	ARG	365		12.811	11.278	1.898	1.00	1.42
MOTA	628	CA	ARG	365	_	11.777	13.151	1.654	1.00	1.36
MOTA	629	HA	ARG	365	_	12.239	13.872	0.997	1.00	1.70
MOTA	630		ARG	365		12.178	13.450	3.100	1.00	1.65
				365		11.321	13.822	3.641	1.00	1.87
MOTA	631	HB1								
MOTA	632	HB2		365		12.535	12.544	3.568	1.00	2.13
MOTA	633		ARG	365		13.286	14.506	3.116	1.00	2.23
ATOM	634	HG1	ARG	365	_	13.961	14.332	2.291	1.00	2.71
ATOM	635	HG2	ARG	365	-	12.848	15.489	3.021	1.00	2.50
ATOM	636	CD	ARG	365	_	14.059	14.415	4.433	1.00	2.72
ATOM	637	HD1		365		14.622	13.494	4.458	1.00	2.80
						14.737	15.253	4.510	1.00	3.17
ATOM	638	HD2		365						
ATOM	639		ARG	365		13.102	14.445	5.574	1.00	3.34
MOTA	640		ARG	365		12.202	14.073	5.468	1.00	3.67
ATOM	641	CZ	ARG	365	-	-13.463	14.966	6.714	1.00	3.90
ATOM	642	NH1	ARG	365	_	-12.721	15.879	7.279	1.00	4.42
MOTA	643	HH11	ARG	365		11.875	16.179	6.838	1.00	4.48
ATOM	644	HH12		365		12.998	16.279	8.153	1.00	4.97
ATOM	645	NH2		365		14.567	14.575	7.290	1.00	4.33
										4.29
ATOM	646	HH21		365		15.136	13.876	6.857	1.00	
ATOM	647	HH22		365		14.844	14.975	8.164	1.00	4.93
ATOM	648		ARG	365	-	-10.254	13.242	1.518	1.00	0.94
A TOM	649	0	ARG	365		-9.739	13.797	0.567	1.00	1.24
ATOM	650	N	CYS	366		-9.529	12.701	2.459	1.00	0.68
ATOM	651	HN	CYS	366		-9.962	12.257	3.217	1.00	0.91
ATOM	652		CYS	366		-8.043	12.759	2.378	1.00	0.77
ATOM	653		CYS .	366		-7.745	13.675	1.890	1.00	1.02
										1.12
ATOM	654		CYS	366		-7.450	12.716	3.787	1.00	
MOTA	655	HB1		366		-6.580	12.076	3.793	1.00	1.32
MOTA	656	HB2	CYS	366		-8.186	12.329	4.476	1.00	1.41
ATOM	657	SG	CYS	366		-6.972	14.387	4.291	1.00	1.97
ATOM	658	HG	CYS	366		-7.177	14.985	3.568	1.00	2.29
ATOM	659		CYS	366		-7.530	11.564	1.572	1.00	0.67
ATOM	660		CYS	366		-7.880	10.430	1.833	1.00	0.66
ATOM	661		LEU	367		-6.705	11.809	0.592	1.00	0.68
ATOM	662		LEU	367		-6.437	12.731	0.397	1.00	0.77
ATOM	663		LEU	367		-6.172	10.689	-0.232	1.00	0.65
ATOM	664	HA	LEU	367		-6.992	10.170	-0.707	1.00	0.65
ATOM	665	CB	LEU	367		-5.235	11.247	-1.303	1.00	0.79
MOTA	666	HB1	LEU	367		-4.373	11.692	-0.831	1.00	1.21
ATOM	667	HB2		367		-5.757	11.995	-1.883	1.00	1.27
MOTA	668		LEU	367		-4.782	10.113	-2.222	1.00	1.20
ATOM	669		LEU	367		-4.447	9.278	-1.624	1.00	1.65
MOTA	670	CD1		367		-5.951	9.673	-3.105	1.00	1.87
MOTA		HD11		367		-6.575	10.525	-3.327	1.00	2.32
MOTA		HD12		367		-6.533	8.926	-2.585	1.00	2.43
ATOM		HD13		367		-5.570	9.256	-4.025	1.00	2.19
ATOM	674	CD2		367		-3.634	10.606	-3.103	1.00	1.50
MOTA	675	HD21	LEU	367		-3.857	10.392	-4.138	1.00	1.88
MOTA	676	HD22	LEU	367		-2.722	10.104	-2.819	1.00	1.84
ATOM				367		-3.513	11.672	-2.974	1.00	2.01
MOTA	678		LEU	367		-5.403	9.715	0.663	1.00	0.56
ATOM	679			367		-5.581				
			LEU				8.515	0.586	1.00	0.53
ATOM	680		ARG	368		-4.551	10.220	1.516	1.00	0.56
MOTA	681	HN	ARG	368		-4.425	11.191	1.564	1.00	0.62
MOTA	682	CA	ARG	368		-3.772	9.323	2.422	1.00	0.51
MOTA	683	HA	ARG	368		-3.041	8.768	1.846	1.00	0.50
ATOM	684	CB	ARG	368		-3.053	10.167	3.477	1.00	0.58
ATOM	685	HB1		368		-3.231	9.746	4.456	1.00	1.21
ATOM	686	HB2		368		-3.431	11.179	3.446	1.00	0.95
ATOM	687		ARG	368		-1.550	10.173			
MOTA	688	HG1		368				3.193	1.00	1.39
ATOM	689					-1.368	10.626	2.230	1.00	1.89
		HG2		368		-1.180	9.158	3.190	1.00	2.10
ATOM	690		ARG	368		-0.830	10.978	4.276	1.00	1.56
ATOM	691	HD1		368		0.130	10.529	4.480	1.00	2.12
MOTA	692	HD2		368		-1.425	10.981	5.177	1.00	1.61
MOTA	693	NE	ARG	368		-0.634	12.378	3.804	1.00	2.27

MOTA	694	HE ARG	368	-1.079	12.686	2.987	1.00	2.72
ATOM	695	CZ ARO		0.130	13.193	4.478	1.00	2.82
ATOM	696	NH1 ARG		0.010	13.279	5.775	1.00	3.23
							1.00	3.31
MOTA		HH11 ARC		-0.668	12.720	6.253		
MOTA	698	HH12 ARG		0.596	13.904	6.291	1.00	3.77
MOTA	699	NH2 ARG	₃ 368	1.014	13.923	3.854	1.00	3.43
ATOM	700	HH21 ARG	3 368	1.105	13.858	2.861	1.00	3.61
MOTA		HH22 ARG		1.600	14.548	4.370	1.00	3.97
	702			-4.721	8.343	3.116	1.00	0.47
ATOM					7.218	3.391	1.00	0.42
MOTA	703	O ARG		-4.368				
MOTA	704	N GL		-5.926	8.758	3.395	1.00	0.51
ATOM	705	HN GL	J 369	-6.199	9.669	3.160	1.00	0.55
ATOM	706	CA GL	J 369	-6.886	7.839	4.065	1.00	0.51
ATOM	707	HA GL		-6.457	7.486	4.991	1.00	0.52
ATOM	708	CB GL		-8.193	8.580	4.354	1.00	0.59
				-8.985	8.162	3.751	1.00	0.79
MOTA	709	HB1 GL						
MOTA	710	HB2 GL		-8.073	9.628	4.117	1.00	1.16
MOTA	711	CG GL		-8.549	8.428	5.834	1.00	1.21
ATOM	712	HG1 GL	U 369	-7.644	8.399	6.421	1.00	1.98
MOTA	713	HG2 GL	J 369	-9.102	7.511	5.978	1.00	1.67
ATOM	714	CD GL		-9.404	9.616	6.280	1.00	1.53
ATOM	715	OE1 GL		-10.074	9.492	7.292	1.00	2.22
	716	OE2 GL		-9.375	10.630	5.602	1.00	1.87
ATOM								0.49
MOTA	717	C GL		-7.163	6.648	3.150	1.00	
MOTA	718	O GL		-7.149	5.510	3.575	1.00	0.50
MOTA	719	N AL	A 370	-7.404	6.898	1.893	1.00	0.50
ATOM	720	HN AL	A 370	-7.403	7.823	1.568	1.00	0.51
ATOM	721	CA AL		-7.670	5.776	0.953	1.00	0.52
ATOM	722	HA AL		-8.472	5.163	1.337	1.00	0.55
ATOM	723			-8.059	6.334	-0.417	1.00	0.59
ATOM	724	HB1 AL		-7.938	7.407	-0.415	1.00	1.16
ATOM	725	HB2 AL		-9.090	6.089	-0.626	1.00	1.02
ATOM	726	HB3 AL	A 370	-7.425	5.901	-1.176	1.00	1.17
ATOM	727	C AL	A 370	-6.402	4.933	0.820	1.00	0.46
ATOM	728	O AL		-6.425	3.727	0.969	1.00	0.44
ATOM	729	N GL		-5.291	5.562	0.551	1.00	0.45
ATOM	730			-5.292	6.536	0.442	1.00	0.48
ATOM	731	CA GL		-4.021	4.799	0.421	1.00	0.41
ATOM	732	HA GL		-4.127	4.049	-0.352	1.00	0.42
ATOM	733	CB GL		-2.880	5.754	0.061	1.00	0.45
ATOM	734	HB1 GL	N 371	-2.031	5.185	-0.287	1.00	0.89
ATOM	735	HB2 GL		-2.598	6.324	0.935	1.00	0.83
ATOM	736	CG GL		-3.336	6.709	-1.045	1.00	0.79
	737			-3.604	7.661	-0.611	1.00	1.41
ATOM		HG1 GL						
ATOM	738	HG2 GL		-4.194	6.289	-1.551	1.00	1.47
MOTA	739	CD GL		-2.199	6.910	-2.048	1.00	1.42
MOTA	740	OE1 GL		-2.220	6.354	-3.128	1.00	2.12
MOTA	741	NE2 GL	N 371	-1.199	7.688	-1.735	1.00	2.08
ATOM	742	HE21 GL	N 371	-1.181	8.138	-0.865	1.00	2.32
MOTA	743	HE22 GL		-0.464	7.821	-2.370	1.00	2.71
ATOM	744	C GL		-3.718	4.117	1.755	1.00	0.37
	745			-3.287	2.982	1.798	1.00	0.35
ATOM		O GL						
ATOM	746	N TY		-3.955	4.794	2.849	1.00	0.38
MOTA	747	HN TY		-4.315	5.705	2.798	1.00	0.41
MOTA	748	CA TY		-3.693	4.167	4.172	1.00	0.38
MOTA	749	HA TY		-2.712	3.713	4.167	1.00	0.37
MOTA	750	CB TY	R 372	-3.766	5.221	5.278	1.00	0.43
MOTA	751	HB1 TY		-4.797	5.391	5.549	1.00	0.46
ATOM	752	HB2 TY		-3.326	6.142	4.929	1.00	0.45
ATOM	753	CG TY		-3.004	4.730	6.483	1.00	0.43
ATOM	754	CD1 TY		-3.630	3.899	7.420	1.00	1.25
MOTA	755	HD1 TY		-4.662	3.611	7.282	1.00	2.15
MOTA	756	CD2 TY		-1.667	5.103	6.661	1.00	1.32
MOTA	757	HD2 TY	R 372	-1.185	5.744	5.938	1.00	2.21
ATOM	758	CE1 TY		-2.918	3.442	8.535	1.00	1.26
ATOM	759	HE1 TY		-3.400	2.800	9.258	1.00	2.15
ATOM	760	CE2 TY		-0.955	4.647	7.776	1.00	1.34
ATOM	761							
		HE2 TY		0.077	4.935	7.912	1.00	2.24
ATOM	762	CZ TY		-1.580	3.816	8.713	1.00	0.51
MOTA	763	OH TY		-0.878	3.366	9.812	1.00	0.57
MOTA	764	HH TY		-1.260	3.771	10.594	1.00	0.96
MOTA	765	C TY		-4.749	3.094	4.416	1.00	0.38
ATOM	766	O TY		-4.512	2.119	5.100	1.00	0.39
ATOM	767	N SE		-5.913	3.260	3.848	1.00	0.40
ATOM	768	HN SE		-6.079	4.049	3.290	1.00	0.42
MOTA	769							
		CA SE		-6.978	2.240	4.033	1.00	0.43
MOTA	770	HA SE	R 373	-7.177	2.110	5.087	1.00	0.45

MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	771 772 773 774 775 776 777	CB HB1 HB2 OG HG C	SER SER SER SER SER SER SER	373 373 373 373 373 373 373	-8.253 -8.878 -7.997 -8.948 -9.193 -6.490 -6.780	2.689 1.828 3.162 3.619 4.371 0.921 -0.145	3.317 3.123 2.384 4.138 3.592 3.437 3.937	1.00 1.00 1.00 1.00 1.00 1.00	0.48 1.00 0.75 1.18 1.47 0.41
ATOM	778	N O	MET	374	-5.732	0.992	2.377	1.00	0.38
MOTA	779	HN	MET	374	-5.502	1.867	1.999	1.00	0.38
MOTA	780	CA	MET	374	-5.200	-0.249	1.749	1.00	0.36
ATOM ATOM	781 782	HA CB	MET MET	374 374	-5.998 -4.614	-0.967 0.110	1.632 0.365	1.00	0.39
ATOM	783	HB1		374	-4.139	1.078	0.424	1.00	0.38
MOTA	784		MET	374	-5.416	0.155	-0.356	1.00	0.40
MOTA	785	CG	MET	374	-3.580	-0.932	-0.098	1.00	0.35
ATOM ATOM	786 787		MET MET	374 374	-2.719 -3.274	-0.894 -0.708	0.553 -1.109	1.00 1.00	0.76 0.77
ATOM	788	SD	MET	374	-4.304	-2.589	-0.043	1.00	1.06
MOTA	789	CE	MET	374	-5.776	-2.214	-1.020	1.00	0.38
ATOM	790		MET	374	-5.989	-3.043	-1.679	1.00	1.01
ATOM ATOM	791 792	HE2	MET MET	374 374	-5.602 -6.613	-1.326 -2.048	-1.606 -0.356	1.00 1.00	1.16 1.05
ATOM	793	C	MET	374	-4.116	-0.828	2.666	1.00	0.33
MOTA	794	0	MET	374	-4.136	-1.991	3.018	1.00	0.37
MOTA	795 796	N	LEU	375 375	-3.173	-0.017 0.916	3.048 2.749	1.00	0.31
ATOM ATOM	797	HN CA	LEU	375 375	-3.183 -2.079	-0.496	3.936	1.00	0.32
MOTA	798	HA	LEU	375	-1.630	-1.382	3.512	1.00	0.32
MOTA	799	CB	LEU	375	-1.023	0.611	4.046	1.00	0.33
ATOM ATOM	800 801		LEU LEU	375 375	-0.468 <b>-1.51</b> 6	0.483 1.572	4.962 4.060	1.00	0.39
ATOM	802	CG	LEU	375	-0.049	0.556	2.850	1.00	0.29
ATOM	803	HG	LEU	375	0.693	-0.208	3.028	1.00	0.34
ATOM	804		LEU	375	-0.797	0.246	1.545	1.00	0.31
ATOM ATOM		HD11 HD12		375 375	-1.039 -0.171	-0.806 0.497	1.513 0.703	1.00	1.12
MOTA	807			375	-1.706	0.827	1.504	1.00	1.03
ATOM	808		LEU	375	0.643	1.912	2.704	1.00	0.32
ATOM ATOM	809	HD21 HD22		375 375	1.428 -0.078	1.998 2.702	3.439 2.852	1.00	0.98
ÄTOM	811		LEU	375	1.067	1.994	1.713	1.00	1.10
ATOM	812	С	LEU	375	-2.648	-0.821	5.319	1.00	0.36
ATOM ATOM	813 814	N	LEU ALA	375 376	-2.103 -3.746	-1.619 -0.213	6.055 5.673	1.00 1.00	0.40
MOTA	815	HN	ALA	376	-4.172	0.423	5.061	1.00	0.37
ATOM	816		ALA	376	-4.357	-0.490	7.002	1.00	0.43
MOTA	817	HA	ALA	376	-3.584	-0.758	7.707	1.00	0.46
ATOM ATOM	818 819	CB HB1	ALA ALA	376 376	-5.088 -5.716	0.761 1.146	7.495 6.705	1.00	0.48
MOTA	820		ALA	376	-4.365	1.512	7.778	1.00	1.10
MOTA	821		ALA	376	-5.698	0.508	8.350	1.00	1.17
MOTA MOTA	822 823	С 0	ALA ALA	376 376	-5.350 -5.228	-1.647 -2.666	6.867 7.520	1.00	0.43
ATOM	824	N	THR	377	-6.332	-1.499	6.018	1.00	0.42
MOTA	825	HN	THR	377	-6.409	-0.672	5.498	1.00	0.43
MOTA MOTA	826 827	CA HA	THR THR	377 377	-7.331 -7.907	-2.590 -2.711	5.832 6.737	1.00	$0.44 \\ 0.48$
MOTA	828	СВ	THR	377	-8.267	-2.236	4.673	1.00	0.46
MOTA	829	HB	THR	377	-7.690	-2.116	3.769	1.00	0.60
MOTA MOTA	830 831		THR THR	377 377	-8.948 -8.501	-1.025	4.966	1.00	0.73
MOTA	832		THR	377 377	-9.282	-0.313 -3.362	4.502 4.473	1.00 1.00	0.87
MOTA	833	HG21	THR	377	-9.052	-3.896	3.563	1.00	1.30
MOTA		HG22		377	-10.275	-2.943	4.405	1.00	1.28
MOTA MOTA	836	HG23 C	THR THR	377 377	-9.234 -6.603	-4.042 -3.895	5.311 5.510	1.00	1.34 0.41
MOTA	837	ŏ	THR	377	-7.045	-4.968	5.864	1.00	0.46
MOTA	838	N	TRP	378	-5.489	-3.809	4.840	1.00	0.36
MOTA MOTA	839 840	HN CA	TRP TRP	378 378	-5.150 -4.730	-2.932	4.564	1.00	0.35
ATOM	841	HA	TRP	378 378	-4.730 -5.351	-5.041 -5.689	4.495 3.895	$1.00 \\ 1.00$	0.36
MOTA	842	CB	TRP	378	-3.478	-4.657	3.704	1.00	0.34
MOTA MOTA	843 844	HB1 HB2	TRP TRP	378 378	-2.856	-4.015	4.309	1.00	0.36
MOTA	845	CG	TRP	378 378	-3.768 -2.717	-4.134 -5.890	2.805 3.337	1.00	0.34
MOTA	846	CD1	TRP	378	-2.033	-6.669	4.207	1.00	0.46
MOTA	847	HD1	TRP	378	-1.951	-6.501	5.271	1.00	0.54

Figure 8 (12 of 19)

MOTA	848	CD2	TRP	378	-2.547	-6.497	2.023	1.00	0.33
ATOM	849	NE1	TRP	378	-1.455	-7.715	3.510	1.00	0.49
MOTA	850	HE1	TRP	378	-0.906	-8.423	3.907	1.00	0.57
ATOM	851		TRP	378	-1.743	-7.652	2.162	1.00	0.40
ATOM	852		TRP	378	-3.008	-6.160	0.738	1.00	0.31
						-5.283	0.601	1.00	0.32
MOTA	853	HE3	TRP	378	-3.624				
MOTA	854	CZ2	TRP	378	-1.408	-8.446	1.064	1.00	0.41
MOTA	855	HZ2	TRP	378	-0.793	-9.323	1.196	1.00	0.48
ATOM	856	CZ3	TRP	378	-2.673	-6.956	-0.369	1.00	0.35
ATOM	857	HZ3	TRP	378	-3.033	-6.688	-1.352	1.00	0.39
ATOM	858		TRP	378	-1.874	-8.097	-0.206	1.00	0.38
ATOM	859		TRP	378	-1.620	-8.705	-1.061	1.00	0.42
ATOM	860	C	TRP	378	-4.325	-5.766	5.781	1.00	0.42
				378	-4.720	-6.888	6.025	1.00	0.48
ATOM	861	0	TRP					1.00	0.45
MOTA	862	N	ARG	379	-3.543	-5.132	6.611		
MOTA	863	HN	ARG	379	-3.237	-4.225	6.400	1.00	0.43
MOTA	864	CA	ARG	379	-3.116	-5.786	7.881	1.00	0.56
MOTA	865	HA	ARG	379	-2.458	-6.612	7.657	1.00	0.60
MOTA	866	CB	ARG	379	-2.378	-4.769	8.753	1.00	0.61
MOTA	867	HB1	ARG	379	-3.033	-4.426	9.540	1.00	1.05
MOTA	868		ARG	379	-2.074	-3.928	8.146	1.00	0.93
MOTA	869	CG	ARG	379	-1.142	-5.425	9.372	1.00	1.20
ATOM	870	HG1		379	-0.455	-5.709	8.590	1.00	1.69
MOTA	871	HG2		379	-1.441	-6.303	9.927	1.00	1.72
			ARG		-0.457	-4.433	10.314	1.00	1.28
MOTA	872	CD		379				1.00	1.81
MOTA	873	HD1		379	-0.446	-3.454	9.859		
MOTA	874	HD2		379	0.556	-4.755	10.501	1.00	1.54
MOTA	875	NE	ARG	379	-1.206	-4.375	11.600	1.00	1.88
MOTA	876	HE	ARG	379	-1.853	-5.076	11.823	1.00	2.50
MOTA	877	CZ	ARG	379	-1.001	-3.389	12.430	1.00	2.25
MOTA	878	NH1	ARG	379	0.175	-2.829	12.501	1.00	2.62
ATOM	879	HH11	ARG	379	0.920	-3.156	11.920	1.00	2.83
ATOM		HH12		379	0.332	-2.074	13.137	1.00	3.07
ATOM	881	NH2		379	-1.974	-2.962	13.188	1.00	2.89
ATOM		HH21		379	-2.875	-3.390	13.133	1.00	3.20
MOTA		HH22		379	-1.817	-2.207	13.824	1.00	3.36
ATOM	884	C	ARG	379	-4.347	-6.302	8.633	1.00	0.62
APOM	885	ŏ	ARG	379	-4.262	-7.219	9.426	1.00	0.72
a fema	886		ARG	380	-5.489	-5.718	8.393	1.00	0.59
ATOM		N					7.751		0.52
MOTA	887	HN	ARG	380	-5.536	-4.976		1.00	0.52
MOTA	888	CA	ARG	380	-6.721	-6.174	9.097	1.00	
ATOM	889	HA	ARG	380	-6.455	-6.560	10.070	1.00	0.77
ATOM	890	CB	ARG	380	-7.678	-4.993	9.264	1.00	0.76
MOTA	891	HB1	ARG	380	-8.600	-5.198	8.740	1.00	1.26
ATOM	892	HB2		380	-7.223	-4.101	8.857	1.00	0.91
ATOM	893	CG	ARG	380	-7.976	-4.784	10.750	1.00	1.59
ATOM	894		ARG	380	-7.119	-4.336	11.229	1.00	2.10
MOTA	895	HG2	ARG	380	-8.188	-5.738	11.211	1.00	2.23
MOTA	896	CD	ARG	380	-9.185	-3.860	10.906	1.00	2.04
MOTA	897	HD1	ARG	380	-9.722	-3.809	9.971	1.00	2.37
MOTA	898	HD2	ARG	380	-8.850	-2.872	11.183	1.00	2.55
ATOM	899	NE	ARG	380	-10.084	-4.396	11.967	1.00	2.53
ATOM	900	HE	ARG	380	-10.383	-5.328	11.931	1.00	2.83
ATOM	901	CZ	ARG	380	-10.473	-3.623	12.943	1.00	3.11
ATOM	902		ARG	380	-10.311	-4.004	14.181	1.00	3.54
MOTA		HH11		380	-9.888	-4.887	14.381	1.00	3.57
MOTA		HH12		380	-10.609	-3.411	14.929	1.00	4.10
MOTA	905		ARG	380	-11.026	-2.470	12.682	1.00	3.72
ATOM		HH21						1.00	3.88
				380	-11.152	-2.179	11.734		4.28
ATOM	907			380	-11.324	-1.878	13.431	1.00	
MOTA	908	С	ARG	380	-7.410	-7.275	8.283	1.00	0.67
MOTA	909	0	ARG	380	-7.454	-8.421	8.685	1.00	0.75
ATOM	910	N	ARG	381	-7.955	-6.934	7.147	1.00	0.70
MOTA	911	HN	ARG	381	-7.914	-6.003	6.846	1.00	0.75
MOTA	912	CA	ARG	381	-8.652	-7.957	6.314	1.00	0.80
MOTA	913	HA	ARG	381	-9.469	-8.380	6.879	1.00	0.86
MOTA	914	CB	ARG	381	-9.203	-7.295	5.049	1.00	0.94
MOTA	915	HB1	ARG	381	-8.389	-7.058	4.380	1.00	1.35
MOTA	916		ARG	381	-9.725	-6.387	5.316	1.00	1.19
MOTA	917	CG	ARG	381	-10.169	-8.253	4.351	1.00	1.64
MOTA	918		ARG	381	-10.890	-8.621	5.066	1.00	2.21
MOTA	919		ARG	381	-9.616	-9.084	3.937	1.00	2.31
MOTA	920	CD	ARG	381	-10.900	-7.515	3.229	1.00	1.84
MOTA	921		ARG	381	-11.038	-8.180	2.390	1.00	2.15
MOTA	922		ARG	381	-10.314	-6.662	2.919	1.00	1.90
ATOM	923	NE	ARG	381	-10.314 $-12.229$	-7.052	3.720	1.00	2.80
ATOM	924	HE	ARG		-12.229 $-12.322$		4.113	1.00	
221 OL1	144	nr	UM	381	-12.322	-6.160	4.113	1.00	3.22

				2 605	1 00 3 46	
MOTA	925 CZ ARG	381	-13.268 -7.836	3.627	1.00 3.46	
MOTA	926 NH1 ARG	381	-13.493 -8.493	2.522	1.00 4.06	
MOTA	927 HH11 ARG	381	-12.869 -8.396	1.747	1.00 4.12	
MOTA	928 HH12 ARG	381	-14.290 -9.093	2.451	1.00 4.71	
MOTA	929 NH2 ARG	381	-14.082 -7.962	4.639	1.00 3.98	
MOTA	930 HH21 ARG	381	-13.910 -7.457	5.486	1.00 4.01	
ATOM	931 HH22 ARG	381	-14.879 -8.562	4.569	1.00 4.63	
MOTA	932 C ARG	381	-7.676 -9.072	5.925	1.00 0.78	
ATOM	933 O ARG	381	-7.778 -10.186	6.397	1.00 0.88	
MOTA	934 N THR	382	-6.734 <b>-</b> 8.787	5.063	1.00 0.78	
ATOM	935 HN THR	382	-6.668 -7.884	4.690	1.00 0.79	
ATOM	936 CA THR	382	-5.761 -9.841	4.646	1.00 0.86	
ATOM	937 HA THR	382	-6.276 -10.587	4.062	1.00 0.93	
MOTA	938 CB THR	382	-4.652 -9.210	3.794	1.00 1.00	
ATOM	939 HB THR	382	-3.689 -9.477	4.202	1.00 1.30	
ATOM	940 OG1 THR	382	-4.792 -7.796	3.799	1.00 1.82	
MOTA	941 HG1 THR	382	-5.486 -7.562	3.177	1.00 2.07	
MOTA	942 CG2 THR	382	-4.751 -9.726	2.358	1.00 0.85	
	943 HG21 THR	382	-3.761 -9.943	1.984	1.00 1.28	
MOTA	944 HG22 THR	382	-5.214 -8.973	1.736	1.00 1.45	
MOTA		382	-5.348 -10.625	2.339	1.00 1.45	
MOTA			-5.143 -10.491	5.895	1.00 0.93	
ATOM	946 C THR	382		6.701	1.00 0.33	
ATOM	947 O THR	382				
MOTA	948 N PRO	383	-5.318 -11.788	6.025 7.202		
MOTA	949 CA PRO	383	-4.768 -12.507			
MOTA	950 HA PRO	383	-5.068 -12.024	8.117	1.00 1.37	
MOTA	951 CB PRO	383	-5.404 -13.892	7.109	1.00 1.57	
ATOM	952 HB1 PRO	383	-6.305 -13.933	7.702	1.00 1.79	
MOTA	953 HB2 PRO	383	-4.703 - 14.649	7.433	1.00 1.68	
MOTA	954 CG PRO	383	-5.735 -14.068	5.663	1.00 1.80	
MOTA	955 HG1 PRO	383	-6.607 -14.695	5.557	1.00 2.21	
MOTA	956 HG2 PRO	383	-4.894 - 14.508	5.145	1.00 1.98	
MOTA	957 CD PRO	383	-6.026 -12.697	5.111	1.00 1.47	
MOTA	958 HD2 PRO	383	-5.638 -12.605	4.105	1.00 1.54	
ATOM	959 HD1 PRO	383	-7.085 -12.494	5.132	1.00 1.64	
MOTA	960 C PRO	383	-3.243 -12.599	7.112	1.00 1.42	
MOTA	961 O PRO	383	-2.700 -13.420	6.400	1.00 1.88	
MOTA	962 N ARG	384	-2.549 -11.761	7.831	1.00 1.85	
ATOM	963 HN ARG	384	-3.008 -11.107	8.399	1.00 2.26	
MOTA	964 CA ARG	384	-1.061 -11.797	7.792	1.00 2.30	)
MOTA	965 HA ARG	384	-0.732 -12.770	7.458	1.00 2.77	
MOTA	966 CB ARG	384	-0.550 -10.725	6.827	1.00 3.43	
ATOM	967 HB1 ARG	384	0.519 -10.620	6.938	1.00 3.74	
MOTA	968 HB2 ARG	384	-1.030 -9.783	7.049	1.00 3.69	)
ATOM	969 CG ARG	384	-0.871 -11.137	5.388	1.00 4.37	,
MOTA	970 HG1 ARG	384	-0.986 <b>-</b> 10.253	4.778	1.00 4.65	j
MOTA	971 HG2 ARG	384	-1.789 -11.707	5.373	1.00 4.55	;
MOTA	972 CD ARG	384	0.271 -11.990	4.833	1.00 5.29	
ATOM	973 HD1 ARG	384	1.111 -11.949	5.509	1.00 5.62	
ATOM	974 HD2 ARG	384	0.567 -11.610	3.867	1.00 5.43	
ATOM	975 NE ARG	384	-0.185 -13.402	4.692	1.00 6.06	
ATOM	976 HE ARG	384	-0.989 -13.609	4.170	1.00 6.11	
ATOM	977 CZ ARG	384	0.487 -14.364	5.264	1.00 6.93	
ATOM	978 NH1 ARG	384	1.790 -14.311	5.312	1.00 7.58	
ATOM	979 HH11 ARG	384	2.274 -13.533	4.910	1.00 7.49	
MOTA	980 HH12 ARG	384	2.305 -15.048	5.751	1.00 8.31	
MOTA	981 NH2 ARG	384	-0.144 -15.379	5.788	1.00 7.38	
MOTA	982 HH21 ARG	384	-1.143 -15.420	5.752	1.00 7.11	
MOTA	983 HH22 ARG	384	0.371 -16.116	6.227	1.00 8.15	
ATOM	984 C ARG	384	-0.514 -11.526	9.195	1.00 1.73	
MOTA	985 O ARG	384	-1.260 -11.365	10.140	1.00 2.21	
MOTA	986 N ARG	385	0.781 -11.476	9.342	1.00 1.68	
MOTA	987 HN ARG	385	1.369 -11.610	8.569	1.00 2.10	
MOTA	988 CA ARG	385	1.365 -11.218	10.688	1.00 2.09	
ATOM	989 HA ARG	385	0.571 -11.017	11.391	1.00 2.63	
MOTA	990 CB ARG	385	2.152 -12.447	11.146	1.00 3.06	
ATOM	991 HB1 ARG	385	2.872 -12.155	11.146	1.00 3.55	
MOTA	992 HB2 ARG	385	2.666 -12.881	10.301	1.00 3.42	
MOTA	993 CG ARG	385	1.189 -13.476	11.741	1.00 3.42	
ATOM	994 HG1 ARG	385	0.884 -14.170	10.972	1.00 3.74	
ATOM	995 HG2 ARG	385	0.884 -14.170	10.972	1.00 3.74	
ATOM	996 CD ARG	385	1.889 -14.242	12.136	1.00 3.90	
MOTA	997 HD1 ARG	385	1.547 -13.871	13.821	1.00 4.81	
ATOM	998 HD2 ARG	385	2.956 -14.101	12.787	1.00 5.22	
ATOM	999 NE ARG	385	1.568 -15.693	12.752	1.00 5.16	
MOTA	1000 HE ARG	385	0.752 -16.047	13.163	1.00 5.34	
ATOM	1000 HE ANG	385	2.374 -16.491	12.107	1.00 5.22	
		505	2.5/4 10.491	,	1.00 0.20	•

ATOM	1002 NH1 ARG	385	2.062 -16.		1.00 6.85 1.00 6.65
MOTA MOTA	1003 HH11 ARG 1004 HH12 ARG	385 385	1.205 -16. 2.679 -17.		1.00 6.65 1.00 7.64
MOTA	1004 HH12 ARG	385	3.491 -16.	877 12.661	1.00 6.90
MOTA	1006 HH21 ARG	385	3.728 -16.		1.00 6.75
MOTA	1007 HH22 ARG	385	4.110 -17.		1.00 7.68 1.00 1.75
MOTA	1008 C ARG 1009 O ARG	385 385	2.301 -10. 1.934 -8.	907 10.970	1.00 2.29
MOTA MOTA	1009 O ARG 1010 N GLU	386	3.509 -10.		1.00 1.72
ATOM	1011 HN GLU	386	3.785 -11.	109 9.893	1.00 2.03
ATOM	1012 CA GLU	386		075 10.081	1.00 2.15 1.00 2.64
ATOM	1013 HA GLU	386 386		147 10.260 254 11.130	1.00 2.64 1.00 3.20
MOTA MOTA	1014 CB GLU 1015 HB1 GLU	386		464 11.027	1.00 3.64
MOTA	1016 HB2 GLU	386	6.049 -10.	210 10.987	1.00 3.43
MOTA	1017 CG GLU	386		.196 12.530	1.00 4.00 1.00 4.00
ATOM	1018 HG1 GLU 1019 HG2 GLU	386 386		.130 12.447 .329 13.052	$1.00  4.00 \\ 1.00  4.22$
ATOM ATOM	1019 HG2 GLU 1020 CD GLU	386	5.324 -10.		1.00 5.05
MOTA	1021 OE1 GLU	386	5.062 -11.		1.00 5.61
MOTA	1022 OE2 GLU	386	5.863 -10.		1.00 5.55 1.00 1.56
MOTA	1023 C GLU	386 386		.049 8.685 .571 8.497	1.00 1.56 1.00 2.12
MOTA MOTA	1024 O GLU 1025 N ALA	387		.560 7.706	1.00 1.11
MOTA	1026 HN ALA	387	3.514 -9	.941 7.880	1.00 1.61
MOTA	1027 CA ALA	387		.567 6.324	1.00 0.92 1.00 1.12
MOTA	1028 HA ALA 1029 CB ALA	387 387		.284 6.355 .971 5.731	1.00 1.12 1.00 1.44
MOTA MOTA	1030 HB1 ALA	387		.069 5.245	1.00 1.84
ATOM	1031 HB2 ALA	387		.704 6.519	1.00 2.02
MOTA	1032 HB3 ALA	387	5.614 -11		1.00 1.84 1.00 0.77
ATOM ATOM	1033 C ALA 1034 O ALA	387 387		.572 5.455 .669 4.244	1.00 0.70
ATOM	1035 N THR	388		.613 6.060	1.00 0.76
ATOM	1036 HN THR	388	3.552 -7	.549 7.038	1.00 0.83
MOTA	1037 CA THR	388		.616 5.262 .112 4.744	1.00 0.68 1.00 0.72
MOTA MOTA	1038 HA THR 1039 CB THR	388 388		.546 6.196	1.00 0.72
ATOM	1040 HB THR	388		.639 6.104	1.00 1.34
MOTĄ	1041 OG1 THR	388		.012 7.537	1.00 1.54
ATOM	1042 HG1 THR 1043 CG2 THR	388 388		.440 8.074 .257 5.815	1.00 1.90 1.00 1.16
ATOM ATOM	1044 HG21 THR	388		.244 6.093	1.00 1.67
MOTA	1045 HG22 THR	388	0.090 -5	.945 6.335	1.00 1.72
ATOM	1046 HG23 THR	388		.380 4.750	1.00 1.78 1.00 0.54
ATOM ATOM	1047 C THR 1048 O THR	388 388		.960 4.242 .148 3.049	
ATOM	1048 O THR 1049 N LEU	389		.195 4.702	
MOTA	1050 HN LEU	389	4.749 -5	.059 5.668	
MOTA	1051 CA LEU	389 389		.531 3.760 .810 3.156	
MOTA MOTA	1052 HA LEU 1053 CB LEU	389		.818 4.558	
ATOM	1054 HB1 LEU	389	7.238 -4	.541 5.145	1.00 0.87
MOTA	1055 HB2 LEU	389		.090 5.214	
MOTA MOTA	1056 CG LEU 1057 HG LEU	389 389		.116 3.597 .779 2.776	
ATOM	1058 CD1 LEU	389		.844 3.053	1.00 1.13
MOTA	1059 HD11 LEU	389		.018 3.146	
MOTA	1060 HD12 LEU	389 389		630 3.616 986 2.013	
MOTA MOTA	1061 HD13 LEU 1062 CD2 LEU	389		1.749 4.343	
MOTA	1063 HD21 LEU	389	8.712 -2	.577 5.385	1.00 1.68
MOTA	1064 HD22 LEU	389		853 3.913	
MOTA MOTA	1065 HD23 LEU 1066 C LEU	389 389		3.558 4.257 5.587 2.855	
MOTA	1067 O LEU	389		5.323 1.718	1.00 0.43
MOTA	1068 N GLU	390	6.412 -6	5.783 3.353	1.00 0.50
MOTA	1069 HN GLU	390		5.975 4.273	
MOTA MOTA	1070 CA GLU 1071 HA GLU	390 390		7.858 2.522 7.602 2.303	
MOTA	1071 HA GLU	390		3.288	1.00 0.63
MOTA	1073 HB1 GLU	390	6.023 -9	9.653 3.139	1.00 0.99
MOTA MOTA	1074 HB2 GLU 1075 CG GLU	390 390	7.133 -8 8.086 -10	3.995 4.341 0.111 2.772	
MOTA	1075 CG GLU	390		9.521 2.430	1.00 1.76
MOTA	1077 HG2 GLU	390	7.704 -10	0.705 1.955	1.00 1.71
MOTA	1078 CD GLU	390	8.547 -11	L.034 3.902	2 1.00 1.45

MOTA	1079 OE1 GLU	390	8.935 -	-12.152	3.606	1.00	1.95
ATOM	1079 OE1 GEU	390		-10.607	5.044	1.00	2.14
ATOM	1080 CE2 GEU	390	6.245	-7.994	1.215	1.00	0.46
ATOM	1081 C GLU	390	6.763	-7.757	0.142	1.00	0.46
MOTA	1082 0 GEO	391	4.995	-8.361	1.297	1.00	0.44
	1083 N DEC	391	4.591	-8.539	2.172	1.00	0.48
MOTA	1084 AN LEU	391	4.181	-8.495	0.058	1.00	0.41
MOTA		391	4.603	-9.265	-0.572	1.00	0.43
MOTA	1086 HA LEU 1087 CB LEU	391	2.743	-8.865	0.428	1.00	0.45
ATOM		391	2.265	-8.022	0.903	1.00	0.49
MOTA	1088 HB1 LEU 1089 HB2 LEU	391	2.751	-9.705	1.108	1.00	0.47
MOTA MOTA	1099 RB2 REU	391	1.972	-9.239	-0.838	1.00	0.47
ATOM	1090 CG LEU	391	2.668	-9.552	-1.602	1.00	0.76
	1091 NG DEC	391	1.005	-10.383	-0.531	1.00	1.11
MOTA MOTA	1092 CD1 LEU	391	0.001	-9.994	-0.452	1.00	1.62
ATOM	1094 HD12 LEU	391		-10.851	0.402	1.00	1.81
ATOM	1094 HD12 LEU	391		-11.113	-1.326	1.00	1.44
MOTA	1096 CD2 LEU	391	1.185	-8.023	-1.328	1.00	0.85
MOTA	1097 HD21 LEU	391	0.518	-7.688	-0.547	1.00	1.46
MOTA	1098 HD22 LEU	391	0.610	-8.295	-2.199	1.00	1.50
MOTA	1099 HD23 LEU	391	1.870	-7.228	-1.582	1.00	1.36
MOTA	1100 C LEU	391	4.194	-7.159	-0.686	1.00	0.35
MOTA	1100 C LEU	391	4.257	-7.110	-1.898	1.00	0.34
ATOM	1102 N LEU	392	4.149	-6.073	0.038	1.00	0.33
ATOM	1102 H LEU	392	4.109	-6.138	1.015	1.00	0.36
ATOM	1104 CA LEU	392	4.175	-4.736	-0.617	1.00	0.30
ATOM	1105 HA LEU	392	3.376	-4.667	-1.341	1.00	0.30
ATOM	1106 CB LEU	392	4.007	-3.646	0.445	1.00	0.31
ATOM	1107 HB1 LEU	392	4.383	-2.709	0.066	1.00	0.30
MOFA	1108 HB2 LEU	392	4.562	-3.923	1.326	1.00	0.35
ATOM	1109 CG LEU	392	2.527	-3.490	0.807	1.00	0.33
ATOM	1110 HG LEU	392	1.967	-4.321	0.404	1.00	0.41
ATOM	1111 CD1 LEU	392	2.380	-3.464	2.329	1.00	0.45
ATOM	1112 HD11 LEU	392	3.283	-3.068	2.770	1.00	1.16
ATOM	1113 HD12 LEU	392	2.211	-4.467	2.691	1.00	1.11
MOTA	1114 HD13 LEU	392	1.543	-2.837	2.599	1.00	1.10
MOTA	1115 CD2 LEU	392	1.990	-2.177	0.227	1.00	0.28
A#OM	1116 HD21 LEU	392	0.990	-2.003	0.596	1.00	1.06
ATOM	1117 HD22 LEU	392	1.970	-2.239	-0.851	1.00	1.01
MOTA	1118 HD23 LEU	392	2.631	-1.361	0.528	1.00	1.01
MOTA	1119 C LEU	392	5.524	-4.555	-1.317	1.00	0.29
MOTA	1120 O LEU	392	5.638	-3.856	-2.304	1.00	0.30
ATOM	1121 N GLY	393	6.550	-5.182	-0.805	1.00	0.31
MOTA	1122 HN GLY	393	6.433	-5.738	-0.007	1.00	0.32
MOTA	1123 CA GLY	393	7.898	-5.053	-1.428	1.00	0.33
MOTA	1124 HA1 GLY	393	8.629	-5.549	-0.808	1.00	0.37
MOTA	1125 HA2 GLY	393	8.154	-4.007	-1.519	1.00	0.34
MOTA	1126 C GLY	393	7.891	-5.700	-2.813	1.00	0.34
MOTA	1127 O GLY	393	8.163 7.579	-5.059 -6.965	-3.808 -2.892	1.00	0.34
MOTA	1128 N ARG	394	7.359	-7.469	-2.080	1.00	0.37
MOTA	1129 HN ARG	394 394	7.553	-7.403 -7.641	-4.222	1.00	0.39
MOTA	1130 CA ARG 1131 HA ARG	394	8.555	-7.683	-4.625	1.00	0.42
MOTA	1131 HA ARG 1132 CB ARG	394	7.003	-9.060	-4.066	1.00	0.42
MOTA MOTA	1132 CB ARG	394	6.227	-9.228	-4.798	1.00	0.92
MOTA	1134 HB2 ARG	394	6.594	-9.179	-3.073	1.00	1.01
MOTA	1135 CG ARG	394		-10.072	-4.280	1.00	1.21
MOTA	1136 HG1 ARG	394		-10.194	-3.361	1.00	1.76
MOTA	1137 HG2 ARG	394		-9.714	-5.054	1.00	1.89
ATOM	1138 CD ARG	394		-11.418	-4.697	1.00	1.42
MOTA	1139 HD1 ARG	394	8.232	-11.935	-5.341	1.00	1.92
MOTA	1140 HD2 ARG	394		-11.254	-5.227	1.00	1.64
MOTA	1141 NE ARG	394		-12.243	-3.484	1.00	2.11
MOTA	1142 HE ARG	394		-11.808	-2.632	1.00	2.52
ATOM	1142 MD AMO	394		-13.544	-3.555	1.00	2.76
MOTA	1144 NH1 ARG	394		-14.235	-2.536	1.00	3.24
MOTA	1145 HH11 ARG	394		-13.768	-1.700	1.00	3.28
ATOM	1146 HH12 ARG	394		-15.233	-2.591	1.00	3.88
MOTA	1147 NH2 ARG	394		-14.155	-4.646	1.00	3.46
ATOM	1148 HH21 ARG	394		-13.625	-5.426	1.00	3.60
MOTA	1149 HH22 ARG	394		-15.152	-4.701	1.00	4.12
MOTA	1150 C ARG	394	6.654	-6.846	-5.170	1.00	0.36
MOTA	1151 O ARG	394	6.957	-6.667	-6.334	1.00	0.38
MOTA	1152 N VAL	395	5.553	-6.358	-4.671	1.00	0.33
MOTA	1153 HN VAL	395	5.335	-6.508	-3.728	1.00	0.32
MOTA	1154 CA VAL	395	4.634	-5.564	-5.528	1.00	0.33
MOTA	1155 HA VAL	395	4.353	-6.145	-6.394	1.00	0.37

MOTA	1156 CB VA	L 395	3.384	-5.204	-4.725	1.00	0.32
ATOM	1157 HB VA		3.666	-4.607	-3.870	1.00	0.29
MOTA	1158 CG1 VA		2.417	-4.411	-5.606	1.00	0.36
MOTA	1150 CG1 VI		2.979	-3.803	-6.300	1.00	0.97
MOTA	1160 HG12 VA		1.803	-3.775	-4.985	1.00	1.08
ATOM	1161 HG13 VA		1.787	-5.095	-6.155	1.00	1.17
	1162 CG2 V		2.704	-6.489	-4.247	1.00	0.35
MOTA	1162 CG2 VA		2.051	-6.861	-5.023	1.00	1.13
MOTA	1164 HG22 VA		2.126	-6.281	-3.359	1.00	1.00
MOTA	1165 HG23 VA		3.455	-7.231	-4.022	1.00	1.08
MOTA	1165 ng25 VA		5.349	-4.289	-5.976	1.00	0.31
MOTA	1166 C V		5.053	-3.728	-7.012	1.00	0.34
MOTA	1167 O V		6.299	-3.833	-5.204	1.00	0.28
MOTA		รับ 396	6.526	-4.307	-4.376	1.00	0.27
MOTA		EU 396	7.046	-2.602	-5.584	1.00	0.28
MOTA		EU 396	6.355	-1.851	-5.937	1.00	0.29
MOTA MOTA		396	7.812	-2.069	-4.371	1.00	0.26
MOTA	1172 CB LI		8.578	-1.385	-4.702	1.00	0.27
MOTA	1174 HB2 L		8.271	-2.892	-3.845	1.00	0.28
MOTA		EU 396	6.852	-1.339	-3.431	1.00	0.25
MOTA		EU 396	5.961	-1.934	-3.293	1.00	0.27
MOTA	1177 CD1 L		7.533	-1.116	-2.081	1.00	0.27
MOTA	1178 HD11 L		7.377	-0.096	-1.763	1.00	0.89
ATOM	1178 HD11 L		8.592	-1.305	-2.177	1.00	1.01
ATOM	1180 HD13 L		7.112	-1.790	-1.350	1.00	0.97
MOTA	1181 CD2 L		6.477	0.014	-4.036	1.00	0.27
ATOM	1181 CD2 L		7.257	0.731	-3.826	1.00	0.97
MOTA	1183 HD22 L		5.549	0.355	-3.603	1.00	1.11
MOTA	1184 HD23 L		6.361	-0.089	-5.103	1.00	0.99
ATOM		EU 396	8.042	-2.946	-6.692	1.00	0.32
MOTA		EU 396	8.150	-2.253	-7.684	1.00	0.34
ATOM		RG 397	8.772	-4.017	-6.526	1.00	0.34
ATOM		RG 397	8.666	-4.557	-5.715	1.00	0.34
ATOM		RG 397	9.768	-4.420	-7.561	1.00	0.40
MOTA		RG 397	10.582	-3.710	-7.573	1.00	0.41
ATOM		RG 397	10.311	-5.811	-7.228	1.00	0.46
ATOM	1192 HB1 A		10.691	-6.274	-8.127	1.00	0.88
ATOM	1193 HB2 A		9.517	-6.418	-6.818	1.00	0.90
MOTA		RG 397	11.440	-5.687	-6.204	1.00	1.21
ATOM	1195 HG1 A		11.190	-4.923	-5.483	1.00	1.73
ATOM	1196 HG2 A		12.357	-5.419	-6.709	1.00	1.81
MOFA		RG 397	11.626	-7.024	-5.483	1.00	1.32
MOTA	1198 HD1 A		10.791	-7.672	-5.705	1.00	1.65
MOTA	1199 HD2 A		11.676	-6.854	-4.418	1.00	1.83
MOTA	1200 NE A		12.889	-7.666	-5.943	1.00	1.97
ATOM		RG 397	13.550	-7.144	-6.443	1.00	2.54
MOTA		RG 397	13.114	-8.924	-5.679	1.00	2.26
ATOM	1203 NH1 A		12.165	-9.805	-5.842	1.00	2.65
ATOM	1204 HH11 A		11.265	-9.516	-6.168	1.00	3.00
MOTA	1205 HH12 A		12.338	-10.769	-5.640	1.00	2.88
MOTA	1206 NH2 A		14.289	-9.301	-5.253	1.00	2.68
MOTA	1207 HH21 A	RG 397	15.016	-8.626	-5.129	1.00	3.03
MOTA	1208 HH22 A	RG 397	14.461	-10.265	-5.051	1.00	2.94
MOTA	1209 C A	RG 397	9.100	-4.450	-8.938	1.00	0.43
MOTA		RG 397	9.626	-3.935	-9.904	1.00	0.46
MOTA		SP 398	7.941	-5.046	-9.035	1.00	0.45
MOTA		SP 398	7.530	-5.454	-8.242	1.00	0.44
MOTA		SP 398	7.242		-10.351	1.00	0.51
MOTA		SP 398	7.815		-11.039	1.00	0.57
MOTA		SP 398	5.853		-10.165	1.00	0.56
MOTA			5.241		-11.026	1.00	1.02
MOTA	1217 HB2 A		5.394	-5.303	-9.278	1.00	0.99
MOTA		ASP 398	5.978	-7.233	-10.018	1.00	1.21
MOTA	1218 CG A		- 000		<u> </u>		
	1218 CG A 1219 OD1 A	ASP 398	5.076	-7.829	-9.454	1.00	1.79
MOTA	1218 CG F 1219 OD1 F 1220 OD2 F	ASP 398 ASP 398	6.974	-7.829 -7.772	-10.472	1.00	2.00
	1218 CG F 1219 OD1 F 1220 OD2 F 1221 C F	ASP 398 ASP 398 ASP 398	6.97 <b>4</b> 7.103	-7.829 -7.772 -3.683	-10.472 -10.912	1.00 1.00	2.00 0.49
MOTA MOTA MOTA	1218 CG F 1219 OD1 F 1220 OD2 F 1221 C F 1222 O F	LSP 398 LSP 398 LSP 398	6.974 7.103 7.243	-7.829 -7.772 -3.683 -3.455	-10.472 -10.912 -12.097	1.00 1.00 1.00	2.00 0.49 0.54
MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399	6.974 7.103 7.243 6.833	-7.829 -7.772 -3.683 -3.455 -2.728	-10.472 -10.912 -12.097 -10.064	1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45
MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936	-10.472 -10.912 -12.097 -10.064 -9.112	1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43
MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728 6.687	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538	1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43 0.48
MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550	1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43 0.48 0.55
MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N 1227 CB N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399 MET 399 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314 5.700	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319 -0.586	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550 -9.636	1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43 0.48 0.55
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N 1227 CB N 1228 HB1 N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399 MET 399 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314 5.700 5.519	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319 -0.586 0.401	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550 -9.636 -10.031	1.00 1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43 0.55 0.51 0.86
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N 1227 CB N 1228 HB1 N 1229 HB2 N	ASP 398 ASP 398 ASP 398 MET 399 MET 399 MET 399 MET 399 MET 399 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314 5.700 5.519 6.113	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319 -0.586 0.401 -0.507	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550 -9.636 -10.031 -8.640	1.00 1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.48 0.55 0.51 0.86 1.11
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N 1227 CB N 1228 HB1 N 1229 HB2 N 1230 CG N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314 5.700 5.519 6.113 4.385	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319 -0.586 0.401 -0.507 -1.363	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550 -9.636 -10.031 -8.640 -9.585	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.43 0.55 0.51 0.86 1.11
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1218 CG A 1219 OD1 A 1220 OD2 A 1221 C A 1222 O A 1223 N N 1224 HN N 1225 CA N 1226 HA N 1227 CB N 1228 HB1 N 1229 HB2 N 1230 CG N 1231 HG1 N	ASP 398 ASP 398 ASP 398 ASP 398 MET 399	6.974 7.103 7.243 6.833 6.728 6.687 6.314 5.700 5.519 6.113	-7.829 -7.772 -3.683 -3.455 -2.728 -2.936 -1.322 -1.319 -0.586 0.401 -0.507 -1.363 -2.415	-10.472 -10.912 -12.097 -10.064 -9.112 -10.538 -11.550 -9.636 -10.031 -8.640 -9.585	1.00 1.00 1.00 1.00 1.00 1.00 1.00	2.00 0.49 0.54 0.45 0.48 0.55 0.51 0.86 1.11

-2.661

0.29

ATOM 1233 399 3.394 SD MET MOTA 1234 399 3.224 CE MET MOTA 1235 3.734 HE1 MET 399 MOTA 1236 HE2 MET 399 3.660 2.176 MOTA 1237 HE3 MET 399 MOTA 1238 8.045 MET 399 -0.613 -10.489 C 1239 8.121 MOTA MET 399 0 ATOM 1240 ASP 400 9.118 -1.351 -10.384 N MOTA 1241 HN ASP 400 9.042 -2.326 -10.33910.459 MOTA 1242 CA ASP 400 -0.705 -10.330 11.219 10.710 1243 MOTA HA ASP 400 -1.463 -10.206 MOTA 1244 CB ASP 400 11.672 1245 ATOM HB1 ASP 400 9.937 MOTA 1246 400 HB2 ASP 10.693 MOTA 1247 CG ASP 400 -0.912 -12.810 11.672 9.701 -0.948 -13.537 MOTA 1248 OD1 ASP 400 MOTA 1249 OD2 ASP 400 -1.604 -12.966 10.510 MOTA 1250 400 C ASP 1251 11.188 MOTA 0 ASP 400 1252 9.800 -0.024 MOTA N LEU 401 MOTA 1253 401 9.258 -0.841 HN LEU 1254 MOTA 9.813 CA LEU 401 10.077 MOTA 1255 HA LEU 401 8.428 8.523 MOTA 1256 401 CB LEU 1257 MOTA HB1 LEU 401 7.975 -0.059 1258 HB2 LEU MOTA 401 ATOM 1259 CG LEU 401 7.556 MOTA 1260 LEU 7.856 HG 401 ATOM 1261 CD1 LEU 401 6.091 5.548 5.661 ATOM 1262 HD11 LEU 401 ATOM 1263 HD12 LEU 401 MOTA 1264 HD13 LEU 401 6.029 ATOM 1265 CD2 LEU 401 7.726 MOTA 1266 HD21 LEU 401 7.166 8.772 7.361 MOTA 1267 HD22 LEU 401 ATOM 1268 HD23 LEU 401 10.837 ATOM 1269 C LEU 401 10.785 11.773 ATOM 1270 0 LEU 401 ATOM 1271 -0.411Ν LEU 402 11.804 12.796 12.320 MOTA 1272 -0.688 HNLEU 402 MOTA 1273 LEU 402 -0.912 CA MOTA 1274 -1.532 -1.730 HA LEU 402 ATOM 1275 13.846 CB LEU 402 14.518 1276 **MOTA** HB1 LEU 402 -1.064 MOTA 1277 HB2 LEU 402 13.354 -2.37714.639 MOTA 1278 CG LEU 402 -2.576 ATOM 1279 14.834 13.828 HG LEU 402 -1.9951280 MOTA CD1 LEU 402 -3.8191281 HD11 LEU MOTA 402 14.473 -4.685 13.031 MOTA 1282 HD12 LEU 402 -3.955 13.408 MOTA 1283 HD13 LEU 402 -3.694 15.963 15.922 ATOM 1284 CD2 LEU 402 -3.001 MOTA 1285 HD21 LEU 402 -2.826 MOTA 1286 HD22 LEU 402 16.131 -4.052 MOTA 1287 HD23 402 16.770 -2.426 LEU MOTA 1288 С LEU 402 13.468 MOTA 1289 0 LEU 402 13.894 MOTA 1290 GLY 13.550 N 403 13.187 ATOM 1291 GLY HN 403 MOTA 1292 14.176 CA GLY 403 MOTA 1293 HA1 GLY 403 14.315 MOTA 1294 HA2 GLY 403 15.131 MOTA 1295 GLY 403 13.245 C MOTA 1296 GLY 13.673 0 403 MOTA 1297 11.969 Ν CYS 404 2.896 -3.7971.00 0.37 -4.589 MOTA 1298 HN CYS 404 11.651 2.415 1.00 0.37 MOTA 1299 CA CYS 404 10.995 3.363 -2.775 0.33 1.00 MOTA 1300 HA CYS 404 11.229 4.377 -2.488 1.00 MOTA 1301 CB CYS 404 -3.361 9.584 3.310 1.00 0.33 MOTA 1302 HB1 CYS 404 8.876 3.083 -2.578 1.00 0.64 MOTA 1303 HB2 CYS 404 9.538 2.543 -4.1211.00 0.55 MOTA 1304 4.914 SG CYS 404 9.180 -4.097 1.00 0.80 1305 MOTA HG CYS 404 8.241 5.070 -3.9721.00 MOTA 1306 С CYS 404 11.081 2.456 -1.550 1.00 0.28 ATOM 1307 10.943 11.320 0 CYS 404 2.900 -0.4271.00 0.27 MOTA 1308 N LEU 405 -1.750 1.188 1.00 0.27 MOTA 1309 HN LEU 405 11.437 0.847 1.00

MOTA

MOTA

MOTA

1384

1385

1386

OE1

OE2

C

GLU

GLU

GLU

409

409

409

15.856

17.167 13.778 -2.489

-1.575

1.543

3.034

4.480

5.740

1.00

1.00

1.00

1.63

1.75

0.36

ATOM 1389 HN GLU 410 14.027 3.008 4.423 1.00 ATOM 1390 CA GLU 410 14.744 3.678 6.341 1.00 ATOM 1391 HA GLU 410 15.501 3.169 6.921 1.00	0.35 0.34 0.38 0.43 0.43 1.11 0.91	
ATOM 1390 CA GLU 410 14.744 3.678 6.341 1.00 ATOM 1391 HA GLU 410 15.501 3.169 6.921 1.00	0.38 0.43 0.43 1.11	
ATOM 1391 HA GLU 410 15.501 3.169 6.921 1.00	0.43 0.43 1.11	
	0.43 1.11	
	1.11	
	1.23	
	1.87	
ATOM 1397 HG2 GLU 410 16.910 5.295 7.036 1.00	1.90	
	1.74	
	2.28	
	2.35	
	0.35	
ATOM 1402 O GLU 410 13.846 4.401 8.443 1.00	0.38	
ATOM 1403 N ALA 411 12.447 4.331 6.747 1.00	0.32	
ATOM 1404 HN ALA 411 12.300 4.132 5.798 1.00	0.32	
	0.33	
ATOM 1406 HA ALA 411 11.526 5.787 7.972 1.00	0.35	
ATOM 1407 CB ALA 411 10.032 4.825 6.761 1.00	0.32	
ATOM 1408 HB1 ALA 411 10.193 4.295 5.833 1.00 ATOM 1409 HB2 ALA 411 9.761 5.848 6.549 1.00 ATOM 1410 HB3 ALA 411 9.235 4.348 7.313 1.00	1.08	
ATOM 1408 HB1 ALA 411 10.193 4.295 5.833 1.00 ATOM 1409 HB2 ALA 411 9.761 5.848 6.549 1.00	1.12	
ATOM 1410 HB3 ALA 411 9.235 4.348 7.313 1.00	0.93	
ATOM 1411 C ALA 411 11.137 3.827 8.760 1.00	0.35	
ATOM 1412 O ALA 411 10.725 4.202 9.839 1.00	0.41	
	0.35	
ATOM 1414 HN LEU 412 11.773 2.300 7.663 1.00	0.33	
	0.40	
	0.43	
ATOM 1417 CB LEU 412 11.291 0.153 9.049 1.00	0.42	
	0.55 0.42	
1400 GG T TTT 440 40 E40 0 100 7 700 1 00	0.42	
ATOM 1420 CG DEO 412 10.548 0.122 7.703 1.00 ATOM 1421 HG LEU 412 11.140 0.627 6.954 1.00	1.00	
	0.79	
ATOM 1423 HD11 LEU 412 10.766 -1.489 6.301 1.00	1.34	
ATOM 1423 HD11 LEU 412 10.766 -1.489 6.301 1.00 ATOM 1424 HD12 LEU 412 9.274 -1.543 7.238 1.00	1.35	
ATOM 1425 HD13 LEU 412 10.805 -1.990 7.991 1.00	1.42	
ATOM 1426 CD2 LEU 412 9.186 0.814 7.836 1.00	0.82	
ATOM 1426 CD2 LEU 412 9.186 0.814 7.836 1.00 ATOM 1427 HD21 LEU 412 8.762 0.590 8.804 1.00	1.47	
ATOM 1428 HD22 LEU 412 8.524 0.457 7.061 1.00 ATOM 1429 HD23 LEU 412 9.314 1.882 7.736 1.00	1.27	
ATOM 1429 HD23 LEU 412 9.314 1.882 7.736 1.00	1.40	
ATOM 1430 C LEU 412 12.456 1.718 10.620 1.00 ATOM 1431 O LEU 412 12.340 1.393 11.785 1.00	0.44	
ATOM 1431 O LEU 412 12.340 1.393 11.785 1.00 ATOM 1432 N CYS 413 13.577 2.203 10.160 1.00	0.50	
	0.44	
	0.41	
	0.51	
	0.89	
	1.35	
	1.97 1.82	
	2.31	
	2.51	
	1.45	
ATOM 1442 O CYS 413 15.731 4.411 11.846 1.00	2.03	
END		